Investigating transport in a tidally driven coral atoll flow using Lagrangian coherent structures

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Abstract

A field experiment study of flow transport around a coral reef was conducted at Scott Reef, an offshore atoll in the Timor Sea. A drifter deployment was designed based on the insight derived from two Lagrangian data analysis approaches, the finite-time Lyapunov exponent method and the optimized-parameter spectral clustering method, which were used to analyze the predictions of a numerical model. This analysis predicted the formation of a key transport barrier during a critical time of the tidal cycle that separated two bodies of water, one remaining trapped within the lagoon, and one advected offshore; this transport structure had no clear signature upon inspection of the velocity fields and thus the use of Lagrangian methods was crucial. The observed drifter trajectories confirmed the predictions, with the drifters separating into two clusters, one on each side of the transport barrier. The results demonstrate how Lagrangian approaches elucidate the processes governing connectivity and water exchanges between atolls and the surrounding ocean.

Within coral reefs, flow transport influences nutrient exchange, thermal exchange, and biological connectivity (Monismith 2007; Lowe and Falter 2015; Green et al. 2018). Studying the organization of flow transport is thus important to understand reef populations and, furthermore, to determine the resilience of reefs to environmental stressors like those associated with climate change and other anthropogenic activities (Botsford et al. 2009). Throughout the global ocean, strong recent coral bleaching events have been linked to the horizontal advective transport of heat (Heron et al. 2016; Hughes et al. 2018; Xu et al. 2018).

The geometry of coral atolls typically consists of relatively large embayments and narrow entrances, where exchange with the open ocean predominantly occurs. The flows in and around reef systems are usually forced by tides or surface wave breaking at the offshore edge of the reef (Monismith 2007). Understanding transport in these spatio-temporally complex settings is challenging. A promising approach is to use Lagrangian methods developed to identify the key structures governing transport. These structures are broadly referred to as Lagrangian coherent structures (LCS) and often considered to be the “hidden skeleton” of fluid flows (Mathur et al. 2007; Peacock and Haller 2013; Haller 2015).

Allshouse and Peacock (2015), Hadjighasem et al. (2017), and Balasuriya et al. (2018) provide recent reviews of LCS methods. They can be classified into two groups: firstly, set-based methods seeking sets of fluid parcels or tracer trajectories that stay coherent, connected and/or compact over time (Froyland and Padberg-Gehle 2015; Hadjighasem et al. 2016; Schlueter-Kuck and Dabiri 2016) and, secondly, methods seeking the boundaries separating regions with different transport behaviors (Haller 2015). Coral reefs are especially amenable to Lagrangian analysis because their bathymetry and forcing mechanisms are prone to generating robust and persistent LCS.

While there are several examples of diagnostic studies using LCS to interpret data from deployments of drifters (Olascoaga et al. 2013; Jacobs et al. 2014; Beron-Vera et al. 2015; Williams et al. 2015; Rypina et al. 2016), there are very few instances where such approaches have been used prognostically to design and execute field experiments. Haza et al. (2007) and Haza et al. (2010) computed the finite-size Lyapunov exponent (FSLE), fields from model forecasts to plan drifter experiments in the Gulf of La Spezia, Italy, focusing on the
timescales of relative dispersion of particles. They observed that the behavior of the drifter trajectories was qualitatively consistent with the FSLE predictions, yielding high relative drifter dispersion near hyperbolic LCS. The FSLE approach, however, is not as widely considered as another LCS method—the finite-time Lyapunov exponent (FTLE). At smaller spatial scales, which are relevant for atolls, for example, FSLE fields are unreliably sensitive to the temporal resolution of velocity fields (Hadjighasem et al. 2017) and do not distinguish the different spatial scales of a system (LaCasce 2008). Among various LCS detection methods, FTLEs have received considerable attention from scholars, with FTLE ridges usually considered to mark hyperbolic LCS positions (i.e., proxy stable and unstable manifolds of hyperbolic trajectories). In flows with large horizontal velocity shear, however, separation between neighboring trajectories may be due to shear, and, in some cases, can yield FTLE ridges that do not correspond to hyperbolic structures (Haller 2015). Here, we use FTLE to identify candidate transport barriers from high rates of trajectory separation and we loosely refer to them as LCS, without specifying their type (e.g., hyperbolic or shear). Alternative techniques for computing hyperbolic LCS, which naturally identify hyperbolic behavior and distinguish it from the shear, are described in Haller (2015). For investigating short-term behavior of trajectories in flows with high uncertainty, Eulerian methods such as objective Eulerian coherent structures (Serra and Haller 2016; Serra et al. 2020) may be used instead or in addition to Lagrangian techniques. For this study, we restricted the scope to FTLE, as it is widely used and simple to implement, and chose the optimized-parameter spectral clustering as a complimentary, set-based approach because it requires relatively few user-input parameters.

To our knowledge, this was the first field study to have used FTLE or set-based methods to plan drifter deployments. Furthermore, it remains to demonstrate the utility of these methods for coral reefs. As such, in this study, we investigate the application of LCS to Scott Reef, an atoll in the Timor Sea, using two complimentary methods: FTLE and spectral clustering. The Lagrangian analysis was performed on numerical model fields prior to field experiments and used to plan and execute drifter releases, which were targeted to identify the key flow transport structures predicted by the LCS methods.

Field site and numerical model

The study was conducted at Scott Reef, an atoll system located approximately half-way between Australia and Indonesia, as shown in Fig. 1. Scott Reef is comprised of North and South Scott Reef: an almost closed atoll and a crescent-shaped atoll, respectively. South Scott Reef, the focus of this study, shelters a shallow half-lagoon that is 25 km in diameter. As a biodiversity hot spot, it is frequently monitored and hydrographic surveys have been used to augment numerical models (Rayson et al. 2011; Gilmour et al. 2013; Green et al. 2018). The circulation is dominated by the strong barotropic tide associated with its macrotidal regime. The flow, governed by the interaction between bathymetry, the vertical density stratification, and the semi-diurnal tide (Rayson et al. 2011; Green et al. 2018), is driven within a channel located between the western tip of Scott Reef South and Sandy Islet, an emerged patch of land. Our study focused on this channel, about 2.8 km wide, 4.3 km long, and 50 m deep, as highlighted in Fig. 1. The steep bathymetry in the channel, combined with the tidal currents, generates internal waves with peak to trough excursions of up to 100 m (Rayson et al. 2018). The resulting enhanced mixing transports nutrients upwards and into the lagoon via tidal flows (Green et al. 2018). As a semi-enclosed system with complex bathymetry and tidal forcing, Scott Reef serves as a useful case study for LCS analysis.

The Stanford University Nonhydrostatic Terrain-following Adaptive Navier–Stokes solver (SUNTANS, Fringer et al. 2006) was used to model the tidally driven hydrodynamics in South Scott Reef lagoon and the surrounding ocean in three dimensions. Details of the numerical ocean model used for this study, including validation with in situ ocean measurements, can be found in Rayson et al. (2018). For this study, the reef bathymetry was discretized with a triangular unstructured mesh with horizontal resolution of 75 m near Sandy Islet. The vertical resolution was 7 m in the upper layer and 7–10 m in the upper 50 m (the lagoon depth). The model was forced with tides from the Oregon State University global tide solution (Egbert and Erofeeva 2002) and initialized with climatological temperature and salinity stratification from the CSIRO Atlas of Regional Seas data (Ridgway et al. 2002). Atmospheric forcing was neglected as the winds were negligible and the model was run for a short enough period to ignore heating and cooling.

The velocity used for the predictive analysis and the planning before the drifter deployment came from a preexisting model run for 2007, narrowed between 27 September and 30 October. Following the cruise, the model was rerun in a hindcast mode with the corresponding conditions for the 2016 period. Being tidally dominated, the model flows for 2007 and 2016 were, as expected, very similar. For brevity, results are presented for the 2016 model only.

Lagrangian methods

For ease and speed of calculations of both trajectories and FTLEs, the model data were uploaded to a web-based gateway, Trajectory Reconstruction and Analysis for Coherent Structure Evaluation (TRACE, Ameli and Shadden 2019). TRACE uses parallel processing for the Lagrangian computations and can process large data sets that are hosted remotely. More information can be found at http://transport.me.berkeley.edu/trace. For all FTLE calculations, the trajectories were seeded at a
resolution of 0.0002° of latitude and longitude; for all spectral clustering calculations, the trajectories were seeded at a 0.0006° resolution.

The FTLE approach falls under the category of methods seeking boundaries between regions with qualitatively different motion (Haller 2015). FTLEs are based on the differentiation of the flow map obtained from advecting particle trajectories via velocity fields’ data sets. The flow map gradient is used to compute the Cauchy–Green strain tensor and its eigenvalues \( \lambda_i(x_0), i = 1,2 \) for a two-dimensional flow. For a forward-time flow map, the largest eigenvalue, \( \lambda_2 \), yields the largest amount of stretching between neighboring tracer particles and is used to construct the scalar FTLE field at the trajectory release time \( t_0 \) for a chosen finite integration time interval \([t_1 - t_0]\). Locally maximum values of FTLE connected along a curve are commonly referred to as ridges (Shadden et al. 2005; Haller 2015).

In oceanic flows, these structures generally act as the most “repelling” material curves (Hadjighasem et al. 2017) and can be considered to serve as proxy hyperbolic-type LCS and barriers to transport, with the following caveats: these may not necessarily be true material curves and stretching could occur in the direction of, rather than perpendicular to, the ridge.

Nevertheless, with appropriate understanding and caution these maximizing ridges of the FTLE fields computed in forward time can be treated as the finite-time counterparts of the stable invariant manifolds of hyperbolic trajectories. Conversely, FTLE ridges of backward-time calculations identify locally most attracting LCS and treated as proxy unstable manifolds. And, maintaining vigilance (see Supplementary Information Data S1), time-evolving ridges computed sequentially over sliding integration windows may serve to visualize the time evolution of LCS.

The spectral clustering approach to LCS (Hadjighasem et al. 2016) seeks to identify coherent sets isolated within the flow domain. The method partitions particle trajectories into clusters based on the time-average distance and connectivity between trajectories. This yields one or several coherent clusters and an incoherent cluster, or mixing region, filling the background space between the coherent clusters. The trajectories are allocated to clusters according to similarity between trajectories: the elements within a cluster are similar, while being different from the elements of other clusters or from the incoherent background. In other words, intracluster similarity is maximized and intercluster similarity is minimized. The method is based on graph theory and works as follows. First, a similarity matrix \( W \) is constructed using inverse pairwise distances between trajectories. A fixed value \( w \) is substituted for the diagonal elements, where the distances between trajectories are 0. \( W \) is then sparsified by removing all elements with distances larger than a sparsification radius \( r \). Eigenvectors of \( W \) are computed and \( k \) leading eigenvalues are identified that are separated from rest by the eigengap, or largest gap between successive eigenvalues. The \( k+1 \) spectral clusters are then retrieved using perturbation theory (Shi and Malik 2000; von Luxburg 2007) by
applying K-means clustering to the matrix consisting of the leading eigenvectors of $W$.

The original spectral clustering method by Hadjighasem et al. (2016) relies on user-chosen parameters: $r$, the offset $w$ in $W$’s diagonal and the sparsification number quantifying the percentage of trajectories that are cut off from $W$. These parameters affect the eigenvalues of $W$, the values of the eigengap and the resulting number of clusters $k$. To minimize the number of user-input parameters, here we use a slightly modified, optimized-parameter spectral clustering protocol, detailed in Filippi et al. (2021). First, to define $k$, our optimized-parameter spectral clustering uses the normalized eigengap, that is, the eigengap divided by the difference between the largest and the smallest eigenvalues, instead of the absolute eigengap. Second, the method sweeps through $r$ to find the $r$-value corresponding to a peak in normalized eigengaps. Third, it sweeps through increasing values of $w$ until the results become insensitive to further increases in $w$. This procedure automatically identifies optimal parameters within predefined ranges. Finally, to quantify the degree of coherence of the resulting clusters, the clusters are assigned a coherence metric quantifying the retainment of trajectories within the cluster with respect to noise. To do this, end points of trajectories are slightly and randomly perturbed. Trajectories are then advected backwards to the start time to quantify how many lands inside the original cluster. This optimized-parameter spectral clustering thus yields the coherent clusters along with their corresponding coherence metric.

Results

Precruise Lagrangian analysis

As illustrated in Fig. 2a, at high tide around spring tide, the flow starts leaving the lagoon through the channel, and at the turn of the ebb, the flow reverses toward the lagoon. FTLE analysis was carried out using the model surface velocity prior to the field experiment, and the most pronounced FTLE ridges occurred with a trajectory integration time of 6 h, a natural scale for a semi-diurnal tidal forcing. A recurring repelling ridge was detected in the channel during a certain phase of the tide. At high tide, this ridge appears at the southeastern part of the channel, almost normal to it, as highlighted in Fig. 2b (left): this ridge indicates locally maximum rates of expulsion between tracer particles. This transport feature defines a clear, transient boundary between two bodies of water: one remaining within the lagoon and another being expelled offshore over the subsequent 6 h. Over the ebb, the ridge moves progressively more northeastward along the channel and at low tide, the ridge lies offshore of the channel, as shown in the right panel of Fig. 2b (right). The FTLE field closely repeated itself over 3 days of high tides around spring tide: a repelling ridge was detected persistently at the same phases of the tide at an almost identical location, as shown by the ridge superpositions in panel 2 of Fig. 2c. The same 6-h FTLE analysis was carried for sliding 15-min intervals spanning over 3 weeks, to look at the FTLE throughout other tidal phases, and only during the periods of high tide around spring tide were these ridges consistently found, with locations and shapes that repeated themselves each day.

The optimized parameter was run over the same time windows. As shown in Fig. 2d, at high tide, two coherent clusters were present, surrounded by an incoherent background cluster. A first cluster, marked in blue, was located within the channel; the southern boundary of this cluster aligned closely with the repelling FTLE ridge. A second, slightly less coherent cluster marked in dark green was located east of Sandy Islet. At low tide, two different clusters were present, one south of Sandy Islet, to the east of and closely aligned with the repelling FTLE ridge offshore of the channel, and another one west of the repelling FTLE ridge.

LCS-based drifter deployment strategy

To investigate the role of the repelling FTLE ridge in organizing transport around Scott Reef, the following drifter deployment strategy was designed. Around high tide, drifters were released from a ship starting at the exit of the channel and moving progressively southeast along the channel into the lagoon, crossing the ridge and the southern boundary of the coherent blue cluster. The drifters were expected to separate into a northwest group and a southeast group, separated by the ridge, with the northern group leaving the channel over the following 6 h and the southern group remaining in the lagoon. Specifically, drifters were to be released along two 8-km-long arrays parallel to the axis of the channel and roughly orthogonal to the direction of “propagation” of the ridge. To minimize deployment time, the release pattern was a zig-zag connecting the deployment locations as illustrated in Fig. 2c (left).

The field experiment was conducted on 02 October 2016 and 03 October 2016 aboard R/V Solander, operated by AIMS. For repeatability, two deployments were carried out with 9 and 12 drifters, respectively. Because spring tide in October 2016 occurred at night and nocturnal operations were not allowed, the first release happened at high tide before spring tide and the second release at high tide after spring tide. Here, we focus on the second release that comprised more drifters, the results from the first release being similar. In agreement with the experimental strategy described above, the release started at the northwestern-most deployment location at high tide, at 06:15 UTC, and lasted 1.25 h, with the last drifter deployed at 07:30 UTC. The drifters themselves comprised two parts: a surface buoy and a submerged sea anchor. The surface buoy was a cylindrical pipe allowing trackers to stay above waterline and emit position and time signals. The trackers used were SPOT Trace, a commercially available GPS tracker system that was set to emit at 2.5-min intervals. An off-the-shelf parachute-type sea anchor was tied to the surface.
Fig 2. Model velocity data (a) and its subsequent 6-h Lagrangian analysis (b–d) for high (left) and low (right) tide around spring tide on 03 October 2016, at 06:00 and 12:00 UTC respectively. (b) Forward FTLE fields. (c) Periodicity of the normalized forward FTLE ridges for 3 d around spring tide. The numbered blue crosses indicate the drifter release pattern and the locations of the first GPS signal emitted, for each drifter. (d) Optimized-parameter spectral clustering results with coherence metrics. Clusters are differentiated by color with the background cluster in blue-gray.
buoy and immersed at about 2-m deep. The drifters were assembled on-board and deployed right after assembly.

Postcruise Lagrangian analysis

The last drifter having been released at 07:30, we consider this time to be the actual start of the experiment. The Lagrangian analyses were recomputed to account for this shift, with the forward and backward FTLE ridges using a 6-h integration window proceeding and preceding the stated time, respectively, and the spectral clusters being computed for the time window 07:30–13:30. The results are summarized in Fig. 3, which shows velocity (a), forward- and backward-time FTLE ridges (red and green curves in band c), spectral clusters (colored sets in b and c), actual drifters (markers in b), and numerically simulated drifters (markers in c) every 90 min from the start to the end of drifter experiment. Further details on the computations can be found in the Supporting Information Data S1.

At 07:30, the outgoing channel velocity reached 1 meter/second or ms\(^{-1}\) and, in agreement with our pre-cruise analysis, according to our numerical model a repelling FTLE ridge (red curve) was present near the southern end of the channel. This ridge separated waters staying in the lagoon from waters being expelled northward through the channel. As the flow progressed, the ridge moved northwestward through the channel. Closely aligned with this ridge at 07:30 and 09:00 were two coherent spectral clusters, blue and orange, the former containing water being expelled offshore and the latter containing water staying inside the lagoon. Overall, the FTLE and spectral clusters analysis for the 07:30–13:30 time interval is consistent with the pre-cruise Lagrangian analysis performed over the ebb, with the notable exception of the appearance at 07:30 of a clear, orange cluster on the south-eastern side of the FTLE ridge. It is worth noting that starting at 10:30, the alignment between the repelling FTLE ridge and the blue and orange cluster boundary begins to degrade. This is because by this time they are starting to present qualitatively different information. The FTLE ridge reveals where the greatest trajectory separation will occur over the next 6 h, whereas the spectral clusters mark the advected location of coherent material patches previously identified at 07:30. As detailed in the Supporting Information Data S1, the material that originally

Fig 3. Scott reef field experiment: Comparison between observed drifter positions, model velocity and LCS results from the start of the drifter release at (left) 07:30 to (right) 13:30, 6 h after all drifters were in water. The drifter positions are marked by the color of the cluster within which they were initially released. (a) Eulerian velocity fields output by the SUNTANS model. (b) Spectral clusters with coherence metrics, forward (red) and backward (green) FTLE ridges, and experimental drifter positions. (c) Clusters and FTLE ridge from (b) and numerical drifter positions. The spectral clusters were advected from 07:30 to 13:30. FTLEs were recomputed at each start time, keeping a 6-h integration window. The numerical drifters were seeded at 07:30 at the initial positions of their corresponding experimental drifters.
comprised the repelling FTLE ridge at 07:30 is actually progressively drawn onto the green attracting FTLE ridge in the channel.

The experimental drifter trajectories confirmed our predictions. As indicated in Fig. 3b, the first seven drifters (blue markers) were released north of the FTLE ridge and within the blue cluster, whereas drifters 8–12 (orange markers) were released south of the ridge within the orange cluster. Over the subsequent 6 h, the first seven drifters left the lagoon while the last five stayed inside. Perhaps most striking is that drifters 7 (filled blue triangle) and 8 (filled orange triangle) were deployed only 1.3 km apart, but exhibited very different behaviors, consistent with the LCS analysis. As one would expect, the numerical drifters in panel 3 of Fig. 3c display the same qualitative behavior, also splitting into two groups: drifters 1–7 leave the lagoon and drifters 8–12 stay inside. Despite having the same initial conditions as the real drifters, however, the simulated trajectories are not identical with the corresponding real drifters over the full 6 h, most notably outside the channel. A comparison between the observed drifter trajectories and the simulated numerical trajectories is provided in the Supporting Information Data S1. The differences could be due to a non fully Lagrangian design of the real drifters and some windage effects (although wind was very weak), but is perhaps most likely due to being more challenging for the numerical model to reproduce open conditions compared to tidally driven convergent flow within the channel.

A final feature deserving attention is the backward-time FTLE ridge that is nearly aligned with the channel axis at all times (green curve in Fig. 3b,c). This LCS is created by the convergent channel flow illustrated in the first two panels of Fig. 3a and corresponds to the most attracting LCS in the domain. Its attracting tendency is clearly illustrated by the behavior of simulated drifters in Fig. 3c; all except two of the simulated drifters converge onto this attracting ridge. The behavior of the real drifters also reproduced this behavior within the channel where the flow was highly predictable; throughout 07:30 to 10:30 all the blue markers and the red triangle marker in Fig. 3b converge onto the attracting LCS along the center of the channel.

**Discussion**

A targeted drifter experiment was designed and executed to investigate the application and utility of two LCS methods computed from a numerical model, FTLE and spectral clustering, to flow transport in an atoll. Our precruise Lagrangian analysis based on the numerically generated velocity revealed the presence of a robust and persistent repelling transport barrier in the Scott Reef South channel during the ebb around spring tide. This feature manifested itself as a sharp forward-time FTLE ridge separating waters staying within the lagoon from waters leaving the lagoon through the channel. Correspondingly, the spectral clustering analysis revealed the presence of a coherent cluster in the channel just north of the FTLE ridge and containing water parcels leaving the lagoon, and the emergence of a second cluster on the south-eastern side of the ridge containing trapped water. Drifters were deployed on both sides of the predicted repelling ridge’s location and within different coherent clusters. The resulting drifter trajectories behaved as anticipated: drifters split into two sets separated by the ridge and belonging to different spectral clusters. The northern set of drifters left the lagoon.
over the following 6 h, whereas the southern set stayed within. These results demonstrate the utility of the approaches to elucidate and bound key transport structures spatially and temporally. Neither the FLTE ridge nor the spectral clusters had any clear signature in the instantaneous velocity field data presented in Fig. 2a, and it was only by virtue of employing these Lagrangian methods that we could understand the organization of flow transport and plan the drifter deployments.

A key consideration in the pertinence of the LCS approach is the velocity data, whether it is obtained from a numerical model or other sources. There are inherently a lot of discrepancies between velocity output from numerical models and true, observed (in situ) velocity. The model velocity is output from solving a simplified set of equations on a limited grid with imperfect forcing and boundary conditions. The model run used, covering the October 2016 period, did not assimilate observed measurements (from wind, waves or in situ current velocity). In addition, the error between the model and the true velocity may result from velocity interpolation, extrapolation, measurement imprecisions, or any other deterministic source. Therefore, any comparisons between true and simulated velocity fields based on advecting individual fluid particles are guaranteed to produce suboptimal results, as illustrated in the Supporting Information Data S1. Regardless of the velocity errors, however, the overall geometry and temporal behavior of the transport barrier in the model agree with the observed motion of the drifters. In this Scott Reef case study, the repeatability of the tidal forcing over different years in the model suggests that the results from the LCS analysis are robust.

The recurrence of the identified LCS, that is, the transport barrier feature at a certain time of the tidal cycle, as well as the behavior of trajectories on its opposite sides, both point to tides as the ultimate driver. When the tide relaxes, some fluid that has left the lagoon cannot reverse its course through the narrow channel, yielding a transport barrier that divides these two water masses. A similar phenomenon featuring pronounced transport features was recently observed in another tidally driven channel flow, south of Martha’s Vineyard in Cape Cod, Massachusetts (Filippi et al. 2021). This suggests that such tidally recurring barriers may be ubiquitous to tidally driven channel flows. However, the exact shape of the transport barrier, the size of the body of water remaining in the lagoon and the detailed geometries of trajectories on the different sides of the barrier depend on a variety of factors including wind, waves, bathymetry, bottom rugosity, and so on. Here, we take some preliminary steps toward a better understanding of the role of vertical velocity and horizontal divergence in generating the observed transport barrier, but a thorough investigation of all the potential influencing factors is out of our scope. Given the recurrence of the identified LCS, it would be worthwhile to investigate “climatological LCS” (cLCS), following the work of Duran et al. (2018), Gough et al. (2019), Maslo et al. (2020), and Gouveia et al. (2021).

While our data set of numerical velocity does not have the temporal coverage required to perform the cLCS analysis, carrying such investigations as part of future work would enable a robust interannual comparison of the results. Notably, it would be of interest to implement cLCS in a flow where divergence is thought to be important and to compare the insights revealed by the cLCS analysis to the ones resulting from the LCS analysis.

In an atoll with a complex bathymetry, the flow may develop significant vertical velocity and acceleration. These three-dimensional effects in near-surface velocity lead to the convergence/divergence regions responsible for attracting/repelling drifters. It is thus reasonable to anticipate that the observed FTLE ridges and spectral clusters may be partly due to surface convergences/divergences, as suggested by the shrinking of the blue cluster’s area in Fig. 3. Another indication is the uniform distribution of simulated drifters at 07 : 30 that becomes visibly nonuniform by 12 : 00, with the drifter density varying over the domain. The presence of large negative FTLE values may also be due to strong convergence in the model near-surface velocity. To understand the influence of surface convergence on the resulting LCS, we separated the flow into the nondivergent and divergent components using the least-squares procedure following (Rypina et al. 2009), then reiterated the Lagrangian analysis using the nondivergent velocity field. Additional details about the method are provided in the Supporting Information Data S1. To evaluate our approach, the Helmholtz decomposition was performed following the method by Smith (2008) and compared to the output of the least-squares procedure. Further details can be found in the Supporting Information Data S1, along with plots of the divergence and the curl for the original flow field and for the results of the Helmholtz decomposition and of the least-squares procedure. Overall, the results of the Helmholtz decomposition and of the least-squares method were qualitatively similar, which increased our confidence in our approach. Within the channel, the convergence was strongest at high tide (06 : 00 UTC) then progressively diminished throughout the ebb. Divergence/convergence was minimal at low tide (12 : 00 UTC) and divergence increased at 13 : 30 UTC, during the flood. The curl exhibited similar trend, with the strongest magnitudes at high tide, decreasing magnitudes during the ebb (from 06 : 00 to 12 : 00 UTC) and a reversal of direction at the turn of the tide. Note that these calculations are highly sensitive to the interpolation and the discretization of the velocity (Wolfram and Fringer 2013), especially with the complex bathymetry in the domain. In addition, the model vertical resolution near the surface is 7 m and the grid spacing may not reflect the energetic near-surface processes in the upper 2 m. The plots of the vertical velocity output by the SUNTANS model within the channel, shown in the Supporting Information Data S1, were moderately conclusive. Nonetheless, relatively strong downward velocity was observed around high tide (up to −0.0445 m s⁻¹) and during the flood, the velocity was predominantly upward.
To further investigate the role of the three-dimensional effects, the model convergence was compared to the convergence observed from the drifter trajectories. The latter was calculated from the area changes of the triangles formed by consecutive triplets of drifters. A figure and a table are provided in the Supporting Information Data S1. This area change from the observed drifter positions was compared to the area change from simulated numerical tracer positions and to the area change from the model, which was calculated using the Liouville theorem. Additional details and figures are provided in the Supporting Information Data S1. The model exhibited stronger convergence than what was calculated from the drifters, but the time evolution of the area of the drifter-triangles showed a decrease in area nonetheless, indicating convergence. The triangles that included drifter 7 showed rather strong divergence, as shown by the area increase, likely due to drifter 7 slightly reversing its direction toward the lagoon after low tide. The triplet formed by drifters 7–9 showed the strongest divergence, with the area increasing from 1.5 km² to almost 8 km² then decreasing to 0.8 km². With the exception of the triplet 4–6, all other triplets showed noticeable convergence. In the northern batch of drifters, the triangles formed by the triplets between drifters 1 and 5 showed noticeable convergence, with areas decreasing from 0.47–0.50 to 0.01–0.16 km² over the course of the experiment. In the southern batch of drifters, the triangles formed by the triplets between drifters 8 and 12 showed noticeable convergence as well, with areas initially between 1.3 and 1.5 km² decreasing to 0.2–1.0 km². In summary, the model divergence was larger than the observed divergence calculated from the triplets of drifters. Several methods exist for estimating divergence from drifters, including the area change method, the Green theorem method, or the linear least squares method; different methods have different advantages and disadvantages, but all methods generally work well for drifter configurations that include multiple (6 or more) closely spaced drifters, and none work well for small number of drifters aligned into long and narrow filaments (see Rypina et al. 2021 and references therein). In this study, while the exact divergence cannot be computed from the area change of triplets of drifters, there was strong qualitative agreement. This suggests that the drifter behaviors and the spectral clusters were indeed influenced by the three-dimensional effects in the flow.

The FTLE and optimized-parameter spectral clustering analyses were reiterated on the nondivergent flow output by the least-squares procedure. The results are shown in Fig. 4. The nondivergent FTLE differ from the original FTLEs but the repelling ridges are still present in the channel, although further north compared to the full flow. The nondivergent spectral clustering results deviate more notably from their full-flow counterparts, with the domain being partitioned into many clusters, although there is still alignment of a cluster pair with the FTLE ridge within the channel. This additional analysis indicates that while the methods can be complementary, the FTLE, and spectral clustering approaches identify qualitatively different behaviors: the former focuses on the existence of strong attraction and repulsion between neighboring trajectories, whereas the latter focuses on coherence of sets of trajectories. The results indicate that spectral clustering is more sensitive to the presence of surface convergence/divergence.

In conclusion, this study used the LCS analysis to identify a key transport feature for a previously unstudied coral reef system. The deployment focused on the Scott Reef channel and targeted the structure of interest through a drifter release in transects. The drifters separated on either side of the predicted transport barrier and thus successfully confirmed the existence of the LCS. Overall, the experiment serves as the first integrated modeling and field demonstration that the LCS analysis can be reliably used as an operational tool for revealing key flow transport features that are not evident to more traditional, Eulerian approaches.

The flow around the study site is characteristic of coral reefs, with a combination of strong bathymetry and tidal forcing. The occurrence of pronounced transport features at a certain time of the tide may be commonly occurring in tidally driven channel flows, which are quite ubiquitous in fringing reefs and atolls. More broadly, the LCS approach is also applicable to wave-driven flows in coral reef systems (Leclair et al. 2020). Thus, in contrast to many other ocean systems for which the LCS analysis provides limited insight, such as systems without dominant structures or systems that are homogeneous in connectivity, coral reef systems seem to be well suited to such approaches to reveal key transport phenomena.

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Conflict of Interest
None declared.

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