Deep-Sea Research II 85 (2013) 81–95

Contents lists available at SciVerse ScienceDirect

Deep-Sea Research II

journal homepage: www.elsevier.com/locate/dsr2

Investigating transport pathways in the ocean

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ARTICLE INFO

Available online 7 August 2012

Keywords:
Transport
Lagrangian data
Assimilation
Dynamical systems

ABSTRACT

The ocean is a very complex medium with scales of motion that range from thousands of kilometers to the dissipation scales. Transport by ocean currents plays an important role in many practical applications ranging from climatic problems to coastal management and accident mitigation at sea. Understanding transport is challenging because of the chaotic nature of particle motion. In the last decade, new methods have been put forth to improve our understanding of transport. Powerful tools are provided by dynamical system theory, that allow the identification of the barriers to transport and their time variability for a given flow. A shortcoming of this approach, though, is that it is based on the assumption that the velocity field is known with good accuracy, which is not always the case in practical applications. Improving model performance in terms of transport can be addressed using another important methodology that has been recently developed, namely the assimilation of Lagrangian data provided by floating buoys. The two methodologies are technically different but in many ways complementary. In this paper, we review examples of applications of both methodologies performed by the authors in the last few years, considering flows at different scales and in various ocean basins. The results are among the very first examples of applications of the methodologies to the real ocean including testing with Lagrangian in-situ data. The results are discussed in the general framework of the extended fields related to these methodologies, pointing out to open questions and potential for improvements, with an outlook toward future strategies.

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1. Introduction

Understanding transport pathways in the ocean is relevant to a number of important applications. Ocean currents transport physical properties such as temperature and salinity (T, S), chemical properties, pollutants, floating debris, particulate and sediments as well as biological quantities such as phytoplankton, zooplankton, larvae and jelly fish. Being able to understand and predict transport by ocean currents is crucial for climatic applications, for instance for understanding heat transport or pathways of species invasions, as well as for applications for a correct management of the coastal ocean ecosystem and for damage control in case of accidents at sea, such as discharges of pollutants and oil spills.

Direct information on ocean currents are obtained through measurements of various types. In particular, Lagrangian instruments, i.e. floating buoys designed to follow the currents with good approximation, provide useful and direct information on transport both at the ocean surface (drifters) and in the ocean interior (SOFAR, RAFOS and Argo floats). Over the past few decades the world ocean has been sampled by Lagrangian instruments (Lumpkin and Pazos, 2007; Rossby, 2007), providing information on the patterns of mean currents and large scale diffusivity as well as on pathways of exchange between different basins (Bower and Rossby, 1989; Bower et al., 1985). Until recently, the sampling has been mostly targeted toward single drifter launches, in order to maximize coverage and information on large scale currents and mean transport properties. In the last few years, there has been a growing interest in the properties of relative dispersion, which provides information on cluster dispersion and is therefore directly relevant to practical applications regarding the spreading of tracers. Relative dispersion is computed from the statistics of particle pair separation. Earlier studies (Davis, 1985; LaCasce and Bower, 2000; Lacorata et al., 2001) have been limited to information from historical chance pairs, i.e. drifters or floats that were not released together but that got close one to another at some time as they were advected by the currents. Recently, sampling more suitable for relative dispersion studies have been used in a few Lagrangian

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http://dx.doi.org/10.1016/j.dsr2.2012.07.031

experiments, where drifters were launched in pairs and triplets closely separated (order of 1 km). Experiments of this type have been recently performed for instance in the Nordic Sea, Atlantic and Mediterranean Sea (Koszalka et al., 2009; Lumpkin and Elipot, 2010; Schroeder et al., 2011), and they have provided information on relative dispersion at scales ranging from the submesoscale (order of 1 km) to the mesoscale and beyond (order of 100 km). Transport studies have also been recently performed using measurements of near surface velocity from high frequency (HF) and very high frequency (VHF) coastal radars (Haza et al., 2010; Molcard et al., 2009; Shadden et al., 2008). The use of radars is emerging as one of the most suitable avenues to make progress regarding transport processes in coastal areas, given the high spatial resolution (about 1 km–100 m) and the extended range (about 10 km–100 km) of the applications.

Information on transport from observations is extremely useful, but unfortunately they are still very limited in terms of coverage, especially concerning the properties of relative dispersion at submesoscales and in coastal areas. Alternatively, transport studies can be performed based on numerical models. Models are less severely limited than observations, and they can be set up to study specific regions of interest. On the other hand, the computation of transport using models is still very challenging due to some intrinsic and conceptual reasons (Griffa et al., 2004). To understand this, consider the basic equation of Lagrangian transport, i.e. the equation that describes particles advected by the current,

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x},t), \tag{1}$$

where $\mathbf{x}$ represents the positions of Lagrangian particles, and $\mathbf{u}$ is the Eulerian velocity field. The equation shows that the trajectory of a particle, $\mathbf{x}(t)$, is the integral of the velocity $\mathbf{u}$. This implies that even small errors in the prediction of $\mathbf{u}$ tend to accumulate and grow in the prediction of $\mathbf{x}(t)$. Since in practice small errors in the velocity $\mathbf{u}$ of the models are unavoidable, due to incomplete knowledge of forcing, topography, coastline and to the influence of small scale unresolved processes, we can expect that this will result in significantly amplified errors in trajectories. Also, the equation is inherently nonlinear, since $\mathbf{u}$ depends on the position $\mathbf{x}$ and it has the property of being very often chaotic (Aref, 1984). This implies that in the presence of time dependence, trajectories are highly sensitive to initial conditions even for very simple Eulerian flows $\mathbf{u}$.

A number of methods have been put forth in the past decade that have helped increase our skills for Lagrangian transport prediction. Different methods have been suggested for different applications. Methods based on statistical approaches are particularly suited for climatic problems. They consist in separating the mean component of the currents from the turbulent and fluctuating component and parameterizing the turbulent part using stochastic methods whose parameters are estimated from Lagrangian data (Bauer et al., 2002; Griffa, 1996; Veneziani et al., 2005a, 2005b).

Other methods, based on a deterministic approach, are more suited for the understanding of specific events, and they rely on dynamical system tools (Ottino, 1989), assuming that the time evolution of the Eulerian velocity field is correctly known. The main concept here is that stagnation points are the main controlling points of the flow not only in the case of horizontal steady flows but also for time varying ones. Elliptic stagnation points corresponding to vortex centers induce cores that tend to remain coherent in slowly varying flows, while hyperbolic structures, characterized by saddle-like stability properties, are responsible for the stretching and mixing occurring around the cores. Hyperbolicity induced by the turbulent coherent structures create directions in which stretching can cause particles to diverge from the structures along the so-called unstable manifolds as well as to converge along stable manifolds (Ottino, 1989). The stable and unstable manifolds intersect at so-called hyperbolic trajectories the motion of which is central to the understanding of the effect of time dependence on the pathways of Lagrangian particles. There has been a rapid development of these techniques (Wiggins, 2005). In particular, the initial restriction to periodic, infinite-time systems has been overcome by focussing on transient stagnation points, finite-time analogs of stable and unstable manifolds and analysis of finite-time data (Coulliette and Wiggins, 2000; Haller and Poje, 1998; Miller et al., 2002; Poje and Haller, 1999). Lagrangian coherent structures (LCS) such as stable and unstable manifolds and hyperbolic trajectories act as barriers to transport and they help visualize the combined effect of the time variability and geometric features (such as eddies and jets) on transport.

An important consequence of the LCS approach is that even though the motion of a single particle is extremely challenging to reproduce because of the high dependence on initial conditions and on the details of the flow, the description of the general pattern of transport is more robust. If ocean transport is dominated by the main LCSs related to vortices, eddies and jets that act as time-dependent barriers, one can then expect that locating such barriers will provide information on the general fate of a particle launched in a certain area. Details on the specific trajectory might be difficult to determine, but the general behavior of a large number of drifters, or passive tracer fields, is expected to be determined by LCS. Various methods have been proposed to identify LCS, ranging from direct identification in terms of flow invariants (Haller and Poje, 1998) to methods based on local dispersion properties. Finite size Lyapunov exponents (FSLEs, Artale et al., 1997; Aurell et al., 1997) and finite-time Lyapunov exponent (FTLE, Haller, 1997) are most popular approaches (Haza et al., 2008; Olascoaga et al., 2006; d'Ovidio et al., 2004; Poje et al., 2010; Shadden et al., 2008). In this paper we mostly focus on FSLEs, that estimate the hyperbolicity on the basis of relative dispersion, namely how fast particle pairs separate from an initial distance of δ to $r\delta$, where r is a specified factor.

Dynamical system methods appear to have a great potential for practical ocean applications. Nevertheless it is important to point out that they are diagnostic tools, in the sense that their accuracy is directly tied to the accuracy of the Eulerian velocity field $\mathbf{u}(\mathbf{x},t)$. Information on ocean velocities are usually provided by numerical model outputs, and one must assume that the simulated structures are not perfectly realistic, but contain errors. In order to enhance our knowledge of ocean structures and our prediction capability, assimilation methods can be used, that combine information from real-time data with model results. In particular, since we are interested in the Lagrangian flow structure, we can expect that assimilation of Lagrangian data will be especially fruitful.

Lagrangian instruments can be considered as proxies for fluid particles and they provide information on their positions and possibly on other environmental parameters at discrete time intervals (Bauer et al., 2002; LaCasce, 2008). Various methods have been suggested to use Lagrangian data for both velocity reconstruction (Taillandier et al., 2008; Toner et al., 2001) and actual assimilation (Kuznetsov et al., 2003; Molcard et al., 2003; Taillandier et al., 2006a). The former consists of improving the velocity field from off-line circulation model outputs by blending it with the Lagrangian data, while full assimilation implies that the circulation model itself is corrected (often by sequential re-initialization) using the corrected velocity fields and adequately balanced mass fields. Reconstruction can be seen as a first step toward assimilation, but it is also valuable per se, especially for operational purposes, since it is extremely flexible and can be applied to the outputs of any model used in case of an accident or

emergency, even when the model does not have a full assimilation capability.

Two main conceptual avenues have been followed for the reconstruction and assimilation using Lagrangian data. The first avenue is based on estimating velocities along trajectories by finite differences, that is, as the ratio between observed position differences and time increments (Hernandez et al., 1995), and then using these velocities to correct the corresponding model state variable. The second avenue, instead, takes directly into account the Lagrangian nature of the data, by making use of the positions of the floating buoys. This is done introducing an observational operator based on the particle advection equation and correcting the Eulerian velocity field by requiring the minimization of the difference between observed and modeled trajectories (Molcard et al., 2003). This second approach, that we refer to as strictly Lagrangian assimilation, tends to provide better results especially when the interval between observations is of the order of or a sizable fraction of T_L, where T_L is the Lagrangian correlation time scale (Molcard et al., 2003). From the technical point of view, the assimilation has been implemented using several methodologies, including optimal interpolation (Molcard et al., 2003, 2005; Özgökmen et al., 2003), mode decomposition techniques (Toner et al., 2001), Kalman filtering (Ide et al., 2002; Kuznetsov et al., 2003; Salman et al., 2006), variational methods (Kamachi and O'Brien, 1995; Nodet, 2006; Taillandier and Griffa, 2006; Taillandier et al., 2006a) and particle filter methods (Krause and Restrepo, 2009; Salman, 2008a, 2008b). While these methods have been thoroughly tested using synthetic data in the framework of numerical models, applications to in situ data and actual operational testing are still limited.

In this paper we provide a review of work that has been done by the authors together with a number of collaborators based on the two main approaches discussed above; on dynamical system methods and on Lagrangian data assimilation. Examples of applications performed in the last few years are discussed, that consider flows at different scales and in various ocean basins. The results are among the first examples of applications of the methodologies to the real ocean that include the use of in-situ Lagrangian data. While a complete review of the vast and fast evolving fields in which our work is situated is outside the scope of this paper, specific discussions including different contributions and directions are included, and a general outlook of the various approach is provided.

Section 2 focuses on applications of methods from dynamical system theory to investigate transport pathways. Two examples of flows in the Mediterranean Sea are discussed, one in the Adriatic Sea offshore the Gargano Cape (Haza et al., 2007), and the other in the small Gulf of La Spezia in the North-Western Mediterranean (Haza et al., 2010). In both cases, FSLEs are used as main diagnostic tool to study transport pathways. In Section 3, we discuss the scale-dependent nature of relative dispersion from a recent experiment in the Mediterranean Sea in comparison to several other observational and modeling studies. In Section 4, the development of an assimilation method based on a variational approach (LAVA) is briefly reviewed (Taillandier et al., 2006a) and examples of applications are discussed, with special emphasis on a recent application in the Pacific Ocean off Taiwan (Chang et al., 2011). The results presented in Section 2-4 and the main approaches behind them are critically discussed in Section 5, pointing out the existing open questions and challenges. A summary is provided in Section 6.

2. Identifying transport barriers using FSLEs

The LCS separate the domain into regions of initial conditions leading to different advective dynamics. Methods such as flow invariants, or extrema of finite size (FSLE) and finite time (FTLE) Lyapunov exponents have already been tested successfully on realistic ocean models, by supplying the main Lagrangian pathways, effectively highlighting coherent structures in chaotic advection. Of particular importance are the hyperbolic trajectories, which are characterized by the intersection of a stable manifold (inflowing branch) and an unstable manifold (outflowing branch) from a time variable velocity field. It was found that seeding drifters in the vicinity of hyperbolic trajectories leads to a successful reconstruction of the Eulerian fields by covering most of the high kinetic energy features (Poje et al., 2002). It is clear then, that identifying the hyperbolic points of the flow field is the key to optimize the launch of a limited set of drifters.

The FSLE is a finite-time proxy for LCS (Haller and Poje, 1998; Poje and Haller, 1999) and it is quite easy to compute. The local FSLE is a metric quantifying the rate of dispersion of particle-pairs based on their launch location and defined as:

$$\lambda(\mathbf{x},t,\delta_i,r)=\frac{\log(r)}{\tau}, \tag{2}$$

where τ is the time required for a particle pair centered at $\mathbf{x}$ to separate from its initial distance δ_i to the distance $r\delta_i$. It follows that launching particle pairs on a regular array generates an FSLE-map where areas of high λ values correspond to ridges of fast dispersion, such as horizontal shear and inflowing branches of hyperbolic regions. Conversely, the same particle set advected backward in time gives a second FSLE map where high λ values shows ridges of particle convergence, including the outflowing branches. Combining the two maps allows for the identification of the hyperbolic points and their time-dependent locations with subsequent repeat launches.

Here, we summarize two field applications. The first one was in the Adriatic Sea and to our knowledge, it is the first time that FSLEs computed from an operational model have been used in a field experiment, the Dynamics of the Adriatic in Real Time (DART06), in order to guide drifter launches (Haza et al., 2007). The second one is a coastal application in the Gulf of La Spezia and is based on a comparison of FSLE barriers identified from VHF radar measurements to trajectories of in-situ surface drifters (Haza et al., 2010).

2.1. Targeted drifter launches during DART06

In winter and spring, the mean flow in the Adriatic Sea is characterized by a stable Western Adriatic current (WAC) flowing south along the western coast, with the Middle Adriatic and Southern Adriatic Gyres separating around the Palagruza Sill offshore of the Gargano Cape, while intense mesoscale variability occurs in the inter-gyre region. This region displays a saddle-type stagnation point in the frozen field east of the WAC edge, leading to possible hyperbolic trajectories in the Lagrangian frame (Veneziani et al., 2007). In order to maximize coverage in the DART06 area, the ship tracks were centered on the WAC and in the adjacent central part of the basin, and drifter pairs were launched at subsequent times in the inter-gyre boundary offshore of the Gargano Cape, by taking into account the changes in surface winds and forecast ocean velocity outputs from the assimilating Navy Coastal Ocean Model (NCOM).

The FSLE fields were computed based on the NCOM model outputs. The spatial distribution of the Lagrangian transport barriers is typically independent of the FSLE map resolution over a certain threshold, although the ridges are better defined by increasing the drifter launch density. The lower bound (coarsest resolution) typically corresponds to the resolution of the Eulerian velocity field, necessary to capture the shear and strain of the smallest resolvable features. Here FSLEs are computed from pairs

obtained from 5 synthetic trajectories centered on each model grid point. This cross-configuration is composed of 4 particle-pairs launched with an initial relative distance of 0.45 the grid-spacing, and the local FSLE-value is obtained from the fastest separating pair. For this experiment, the launch configuration involved a total exceeding 100,000 particles advected both forward and backward in time from the two-day forecast and two-day hindcast model velocities, respectively. The ratio parameter r was chosen to be 15. In general, the value of the parameter r depends on the integration time and on the domain, but it is typically chosen to be of the order of 10 or more. High ratios of r combined with longer integration times tend to reduce the thickness of the FSLE ridges and improve their definition, even though there is a significant flexibility in the parameter values that allow to capture the structures. Forward time advection identifies particles which diverge when released along inflowing/stable manifolds. Consistent with the commonly used convention in the LCS community, these manifolds are shown in blue and negative values. Conversely, backward time integration is needed to identify the outflowing/unstable manifolds. which are shown in red and positive values (see Fig. 1). Zero-values indicate weak or no dispersion (convergence), since technically, the particle-pairs could not reach the relative distance $r\delta_i$ after the two-day advection period.

The FSLE results were then used in conjunction with the velocity fields themselves to detect a pronounced hyperbolic trajectory (hereafter HT) along the ship tracks. Note that no local FSLE was computed outside of the ship-track domain. Most of the time, the HTs emerge as semi-isolated intersections of opposite FSLE extrema to the east of the WAC, represented by intense overlapping FSLE ridges. A subset of 10–20 synthetic particles were then launched in the in-flowing branches and advected forward in time for two days as a preliminary test, before identifying 2 or 3 drifter launch locations in the vicinity of the HT, which were communicated to the ship on a real-time basis.

Three sets of drifter pairs were launched in March 2006 (Fig. 1), and two sets achieved the expected results, in that the launch targeting the outflowing branches of the HT led successfully to the drifters diverging immediately and being advected in opposite directions (Fig. 1 left and right panels). The success of the launches depended also on optimal wind conditions, minimal delay between predicted and actual launch times due to observational constraints, rapid change in the HT location, and possible model discrepancies. The wind was shown to be a major factor since the HT was not

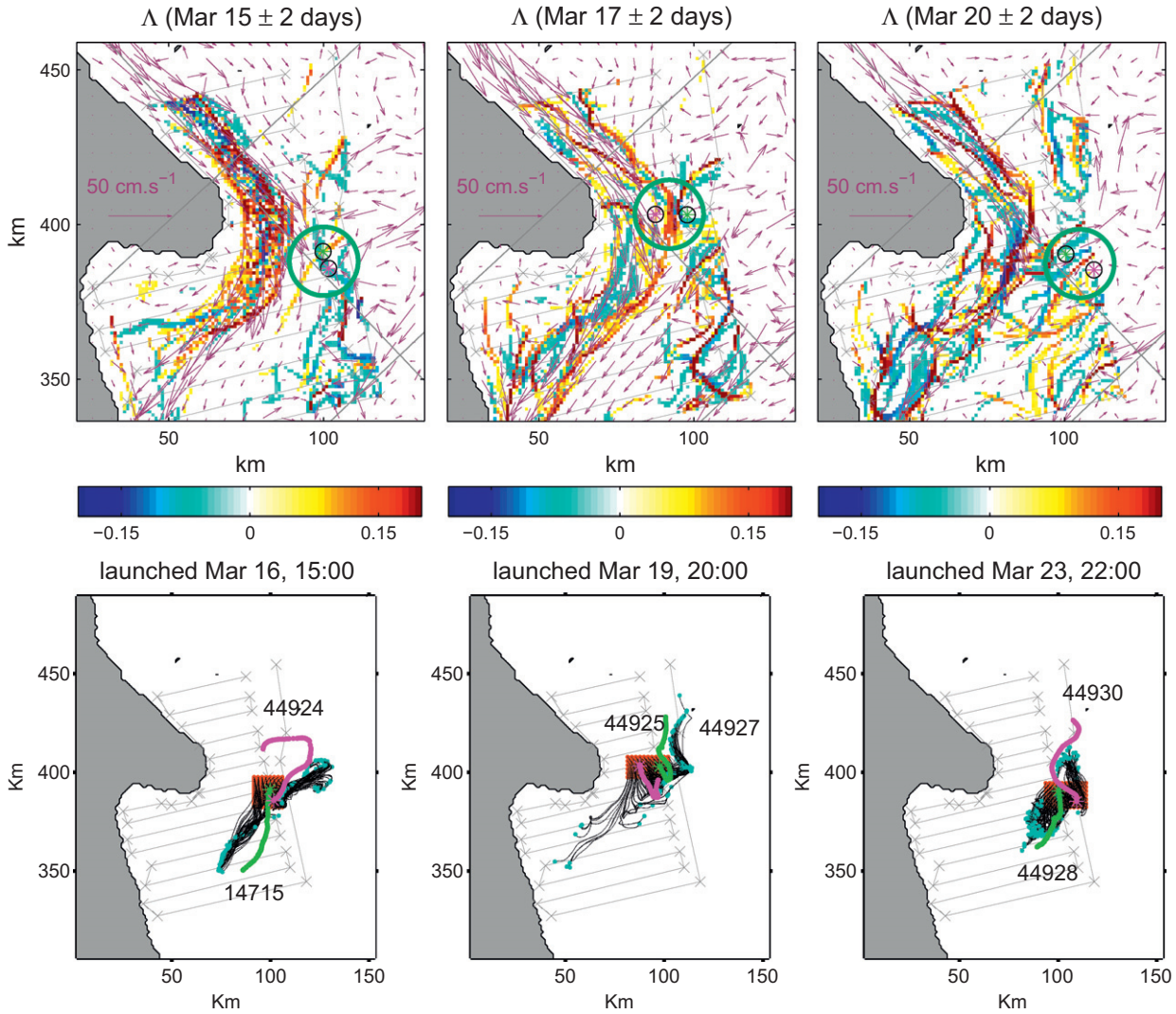

Fig. 1. (Upper panel) FSLE maps computed from the NCOM forecast/hindcast fields in the Adriatic Sea for the predicted launch time. Superimposed are the launch locations of the two real drifters. The colorbar shows the FSLE scale in 1/h. (Lower panel) Trajectories of real drifters (magenta and green) launched during DART06 experiment, superimposed on synthetic trajectories from nearby initial launch positions. The red and cyan dots indicate the initial and final positions of the synthetic trajectories. Adapted from Haza et al., 2007. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

captured in the field following a major wind event (Fig. 1 middle panels). This launch actually acted as an inadvertent "control" experiment in the sense that the circulation model was indeed indicating at the time that the HT was cancelled by the wind, as shown by the FSLE field of the launching day, March 19, depicted in Haza et al. (2007, Fig. 3b). The ship though due to logistic reasons performed the drifter launches in any case, and the observed and numerical trajectories did not show separation.

Overall, this experiment has demonstrated that Lagrangian diagnostics relying on Eulerian fields from accurate operational coastal models can successfully guide real-time directed drifter launches. It also served to increase our confidence that HTs, until then only demonstrated within the context of numerical models, could exist in the real ocean.

2.2. FSLEs from VHF radar during POET-LASIE

One of main goals in this study was to investigate the validity of the Lagrangian transport barriers at the small-scale coastal range. It was part of the Marine Rapid Environment Assessment 2007 (MREA07) in the Ligurian Sea (North Western Mediterranean Sea), during the POET-LASIE component (Gasparini et al., 2009) in the Gulf of La Spezia. The experiment occurred during the last two weeks of June 2007, and involved the measurements of surface velocities from a VHF radar, in conjunction with the release of four drifter clusters.

The Gulf has dimensions of about 5 km by 10 km, with its complex circulation influenced in part by the larger scale Ligurian current, which generates a prevalent cyclonic circulation in the Gulf, and in part by inertial oscillations and variable wind forcing either reinforcing the cyclonic circulation (Scirocco) or disrupting it (Libeccio). Two VHF WERA stations were deployed 7 km apart along the Gulf coast, and supplied surface velocity fields on a rectangular grid with a resolution of 250 m every 30 min. The launch of clusters of CODE surface drifters (Poulain, 2001) allowed for a validation of the radar performance through a direct comparison of radar radial velocities with in-situ drifter velocities, as well as through a qualitative comparison between drifter trajectories and virtual particles advected by the radar velocities with identical initial conditions (Molcard et al., 2009).

The behaviour of the drifter clusters were also used to compare with radar-derived Lagrangian coherent structures and their spatio-temporal evolution (Haza et al., 2010). The FSLE maps were computed from the VHF radar velocities by launching synthetic drifters in a cross-configuration corresponding to four particle pairs centered on a regular grid with a size of 125 m, corresponding to half of the original radar velocity grid, and initial pair separation of 56.25 m. The ensemble of particles (a total of 24,500) were advected both forward and backward in time for 12 h with an integration time-step of 15 min. The launch was then reinitialized every 30 mins. Note that due to the short residence-times of the region, the emergence of visible transport barriers restricted the choice of the distance ratio r to a smaller value of 7, which in turn resulted in thicker ridges of the FSLE extrema. However, increasing the resolution of the FSLE-map to twice the radar grid allowed for better resolved transport barriers. The FSLE-domain was also reduced to exclude regions too close to the coast in order to avoid bias in the spatial interpolation of the radar velocities.

Animation of the FSLE maps and in-situ drifters (http://www.rsmas.miami.edu/personal/ahaza/radar/LaSpezia_fsle_clusters.gif) shows that FSLE extrema appear as a web of ridges evolving in space and time with the flow, consistent with the inertial oscillations and with the main currents. Our initial perception was that these FSLE features were far more complex than those encountered by Shadden et al. (2008) in the Monterey Bay, another circulation observed by HF radars. It seems quite likely that these complex FSLE features are associated with Langmuir cells, arising from the forcing of wind and wave interactions (Craik and Leibovich, 1976; Langmuir, 1938). The drifter motions seem to be controlled by the FSLE ridges, which act as transport barriers even at these scales. Fig. 2 displays several snapshots of two drifter clusters corresponding to different types of relative dispersion. The first cluster is advected with minimal dispersion under the control of the persistent cyclonic flow, which is mainly constrained by two opposite extrema. On the other hand, the second cluster appears to have been released near a hyperbolic point, as displayed by the intersection of two opposite FSLE ridges. About half of the drifters evolve along one outflowing branch (yellow band in Fig. 2 right column), while the other half moves along the other outflowing branch.

As a conclusion, the radar derived flow fields showed that a complex LCS field characterizes the coastal flow in the Gulf of La Spezia. Although single in-situ drifters tend to diverge in time from synthetic ones advected by the velocity field (Molcard et al., 2009), their motions are quite consistent with the spatio-temporal evolution of the transport barriers highlighted by the ridges of FSLE extrema, indicating that these are robust indicators of Lagrangian pathways.

2.3. Extended discussion and outlook

The results presented above are among the first ones to use direct information from in-situ Lagrangian data to test the applicability of LCSs for the detection of transport pathways in the real ocean. Similar results have been shown also by Shadden et al. (2008) using LCSs based on velocities from HF radar data, and by Beron-Vera et al. (2008) and Resplandy et al. (2008) using altimeter based velocities. More recently, Nencioli et al. (2011) used altimetry data as a first guess in a coastal area (where the altimeter is only partially reliable) combining the data with in situ drifters using an adaptive sampling strategy.

While Lagrangian in-situ data provide direct information on instantaneous velocity and transport, tracer data can also be used to validate the presence of LCS in the ocean, since they provide time integrated transport information. Correlations between advected tracers at the ocean surface and altimetry based LCS have been reported for the open ocean in a number of recent papers, such as Abraham and Bowen (2002) and d'Ovidio et al. (2009) for Sea Surface Temperature (SST) and Lehahn et al. (2007) for chlorophyll concentration. LCS computed from local Lyapunov exponents (FSLEs or FLTEs) appear able to reproduce not only barriers of slowly varying features, but in some cases also submesoscale filaments and fronts present in the tracer patterns. Since altimeter based velocity fields are inherently geostrophic and have relatively coarse resolution, they can only resolve the mesoscale field. The agreement between LCS and tracer filaments and fronts is therefore an indication that at least in the considered cases submesoscale phenomena appear mostly due to stirring and advection of mesoscale quasi-2D fields.

The actual nature of submesoscale features is still an open question in the literature. While the indications discussed above suggest that they are non local in nature and induced by the stirring of mesoscale features, other studies (Boccaletti et al., 2007; Müller et al., 2005; Thomas et al., 2008) indicate that submesoscales are in many cases characterized by local dynamics related to frontogenesis and ageostrophic instabilities. They are expected to play an important role in ocean dissipation especially in the surface layers, providing a direct link between slowly evolving quasi-geostrophic mesoscale flows and fast evolving and dissipating 3D processes (McWilliams, 2008).

Direct measurements of submesoscales in the ocean are still limited and challenging, because of the high resolution in space and time required to capture them. A promising avenue to characterize

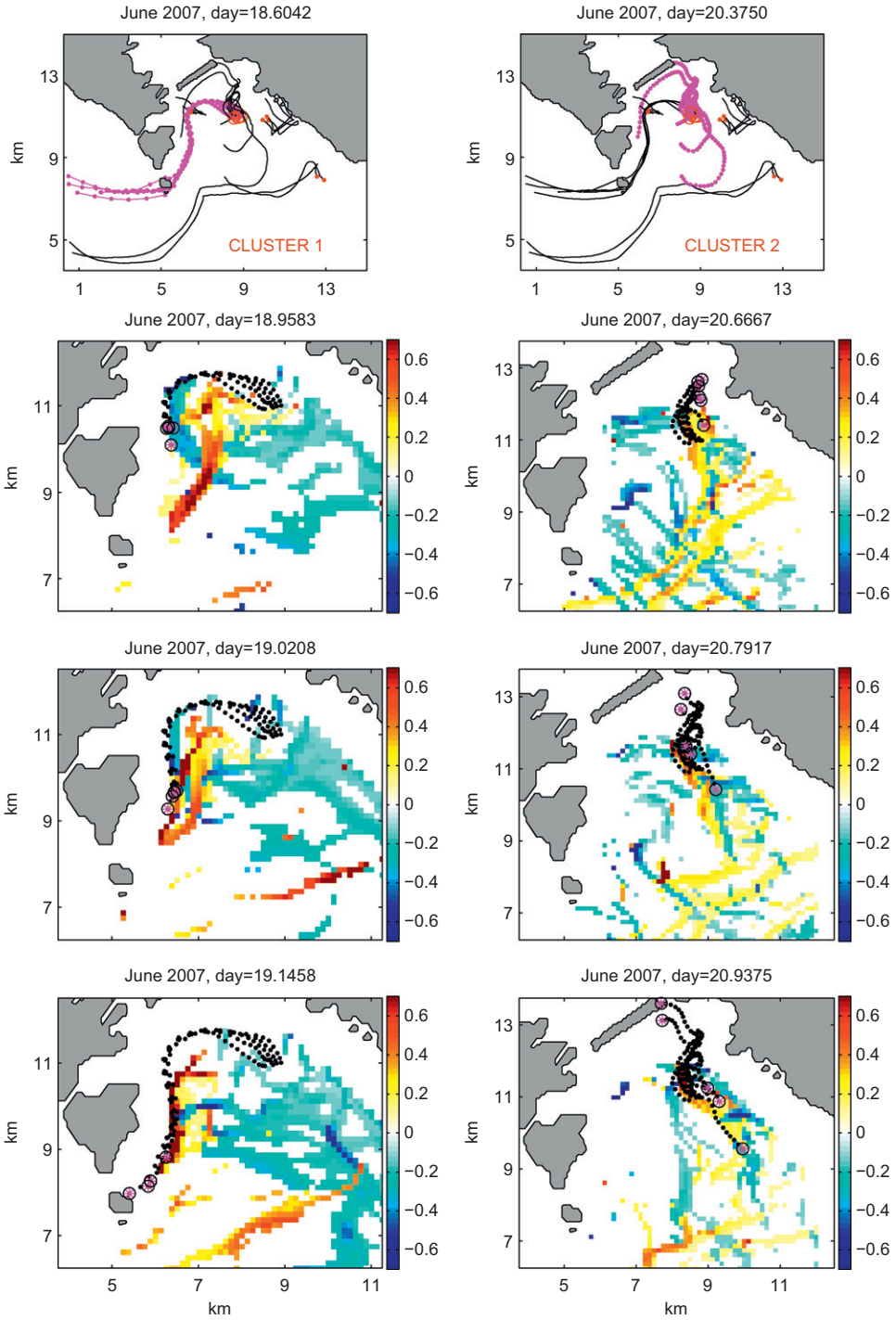

Fig. 2. Upper panels show trajectories of the real drifter clusters launched in the Gulf of La Spezia (Ligurian Sea) during MREA07/POET experiment, with the analyzed clusters in purple (cluster 1 left column, Cluster 2 right column). The other panels show the time evolution of the FSLE field computed from the VHF radar velocities (upper to lower). The color bar indicates FSLE value in 1/day. An animation is available from: http://www.rsmas.miami.edu/personal/ahaza/radar/LaSpezia_fsle_clusters.gif. Adapted from Haza et al., 2010 (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

submesoscales, and in general to quantify the multiscale nature of ocean flows, is given by Lagrangian measurements of relative dispersion. This is discussed in details in the next section.

3. Characteristics of scale-dependent transport

The main question of interest here is the potential influence of motions at different horizontal scales on spreading of drifter clusters (or tracers). One way to address this question is trough measurements of relative dispersion, i.e. dispersion of particle pairs, which is an inherently scale dependent quantity. Several experiments targeted to relative dispersion have been performed in the last few years (Koszalka et al., 2009; Lumpkin and Elipot, 2010; Schroeder et al., 2011), by launching drifters in pairs, triplets or clusters with initial distances of the order of 1 km or less, allowing for multi-scale investigation. Here we provide a brief review of results obtained by an experiment in the

Mediterranean Sea (Schroeder et al., 2011) where the authors were involved, and then we discuss the outcomes in the framework of other findings in the literature.

Clusters of surface drifters have been deployed during two Marine Rapid Environment Assessment (MREA) experiments in the Ligurian Sea in the Northwestern Mediterranean, covering different months in 2007 and 2008, respectively. The clusters have initial radii of less than 1 km, i.e. an order of magnitude below the typical mesoscale deformation radius (approximately 10 km). The data set, consisting of 45 original pairs, has been analyzed computing two independent metrics describing relative dispersion, i.e. mean square separation of particle pairs $D^2(t)$ and FSLEs. Results for $D^2(t)$ computed from the original pairs (i.e. launched at the same time) are shown in Fig. 3 for the combined 2007 and 2008 data set (similar results are obtained for the individual years, not shown). The initial phase is characterized by a straight line in the semi-log plot, indicating an exponential growth for the first ≈ 6 days with an e-folding time scale T_{exp} of approximately 0.5–1 day. A clear regime change occurs after that, but it is difficult to define the nature of the second regime because of the reduced number of original pairs due to drifter mortality. Results for the FSLE diagnostics are shown in Fig. 4, obtained using also chance pairs that provide approximately 50 total pairs in the spatial range between 1 and 200 km. The results indicate an exponential regime, i.e. approximately scale-independent FSLE value or FSLE "plateau", in the submesoscale range of $\approx 1-10$ km, with λ values in the range of 0.7–1.5 days^{-1} consistent with the T_{exp} values in $D^2(t)$ ($\lambda_{max} \approx 1/(2T_{exp})$). At smaller scales, 0.1–1 km, λ seems to gradually increase, but at those scales there is a reduction in the number of pairs and the analysis could contain sampling errors. In the mesoscale range, $\approx 10-100$ km, a power law behavior is obtained with $\lambda(\delta) \approx \delta^{-0.75}$, which is quite consistent with previous studies in the mesoscale indicating regimes between Richarson $\delta^{-2/3}$ (Babiano et al., 1990; Bennett, 1984; Ollitrault et al., 2005; Richardson, 1926)and ballistic δ^{-1} (Haza et al., 2008; Poje et al., 2010).

In summary, the two diagnostics $D^2(t)$ and FSLE show broadly consistent results in the submesoscale, that appears to be characterized by an exponential behavior. This suggests that relative dispersion is predominantly nonlocal, namely controlled mainly by mesoscale dynamics and that the effects of the submesoscale motions are negligible in comparison (Sawford, 2001). Exponential relative dispersion in fact is expected to be linked to a steep

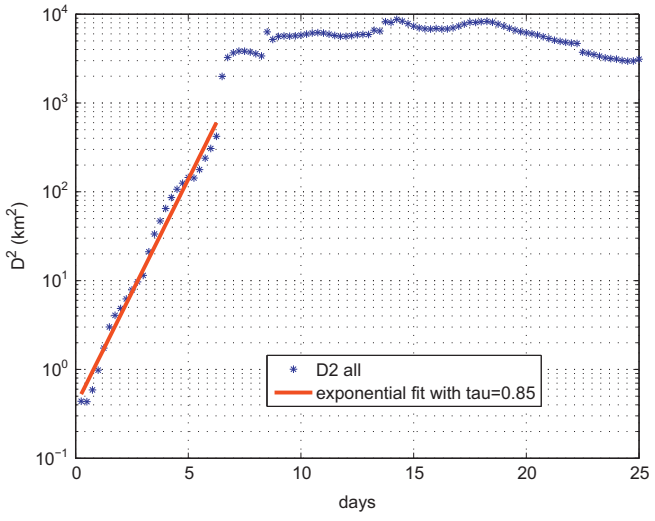

Fig. 3. Relative dispersion in the Ligurian Sea as a function of time in a semi-log plot for all original drifter pairs in 2007 and 2008. Adapted from Schroeder et al. (2011).

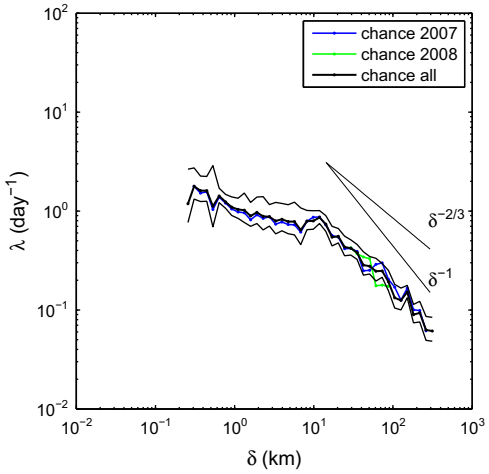

Fig. 4. The Finite Scale Lyapunov Exponent $\lambda(\delta)$ in the Ligurian Sea from all original and chance pairs in 2007 and 2008. The 95% confidence intervals for the combined data set are shown in black thin lines. The slopes corresponding to ballistic $\lambda \sim \delta^{-1}$ and Richardson $\lambda \sim \delta^{-2/3}$ regimes are marked. Adapted from Schroeder et al. (2011).

kinetic energy wave number k spectrum (Bennett, 1984), $k^{-\alpha}$ with $\alpha \geq 3$ in the submesoscale range.

3.1. Extended discussion and outlook

The results in Schroeder et al. (2011) are consistent with findings of other authors based on drifter pairs in the Gulf of Mexico (LaCasce and Ohlmann, 2003) and in the Nordic Seas (Koszalka et al., 2009), where an exponential regime was found in the submesoscale range with T_{exp} of the order of 2–3 days and 0.5 days respectively. An exponential regime with markedly different values has been found from the analysis of HF radar in the Gulf of La Spezia (Haza et al., 2010), characterized by smaller T_{exp} and higher λ. This is likely to be due to geometrical effects in the Gulf, that has dimensions of ≈ 10 km. Remarkably different results have been found by Lumpkin and Elipot (2010) in the region of the Gulf Stream, not only in terms of parameter values but also in terms of regimes. They report a power law extending from the mesoscale to the submesoscale, with a possible exponential behavior occurring only at scales smaller than 1–2 km. This difference could be due to the geographical region, possibly characterized by an active submesocale field influencing transport at various scales, or it might be due to the stormy winter condition during these launches. Also, results by Berti et al., 2011, in the SouthWestern Atlantic show evidence of the existence of multiple regimes occurring at the submesoscale. Finally, model results by Poje et al. (2010) have shown that hyperbolicity tends to increase in model outputs at increasing resolution, but the increase occurs only in the submesoscale range, while mesoscale transport remains unchanged, as shown by a scale dependent FSLE analysis.

We present a list of the characteristics of the FSLE regimes from existing studies in Table 1, as well as all the FSLE curves from observational and modeling studies conducted by the authors of this paper in Fig. 5. These indicate that all models show a clear FSLE plateau over the scale range of the coherent turbulent structures, typically the radius of deformation, while several observations lack such scale-independent behavior and indicate much higher λ_{max} than those obtained in models thus far. It is not clear at this point in time why the differences over the submesoscale regime occur. One possibility is the presence of flow instabilities leading to the formation of active and local submesoscale features (Müller et al., 2005; McWilliams,

Table 1
Comparison of the characteristics of exponential regimes from different studies. Superscript (∗) indicates the estimate from relative dispersion whereas the others from FSLE computation. WAC: (idealized) western Adriatic current, MLI: idealized mixed layer instability.

Data and model (resolution)	Region	λ_{max} (days^{-1})	FSLE plateau	Citation
SCULP drifters	Gulf of Mexico	0.3	$\delta < 20$ km	LaCasce and Ohlmann (2003)
VHF radar	Gulf of La Spezia	4–7	$\delta < 1$ km	Haza et al. (2010)
CLIMODE drifters	Gulf Stream	10	–	Lumpkin and Elipot (2010)
CODE drifters	Ligurian Sea	0.7–1.5	$\delta < 10$ km	Schroeder et al. (2011)
DOLCEVITA drifters	Adriatic Sea	2	–	–
POLEWARD drifters	Nordic Seas	0.5*	$t < 2$ days	Koszalka et al. (2009)
NCOM (1 km)	Adriatic Sea	0.6	$\delta < 10$ km	Haza et al. (2008)
ROMS (0.5 km)	WAC	0.7	$\delta < 4$ km	Poje et al. (2010)
HYCOM (8 km)	Gulf Stream	0.4	$\delta < 50$ km	Poje et al. (2010)
HYCOM (2 km)	Gulf Stream	0.7	$\delta < 10$ km	–
NCOM (0.6 km)	Ligurian Sea	1	$\delta < 10$ km	Schroeder et al. (2011)
LES (5–0.57 m)	MLI	0.3–2	$\delta < 1$ km	Özgökmen et al. (2011)

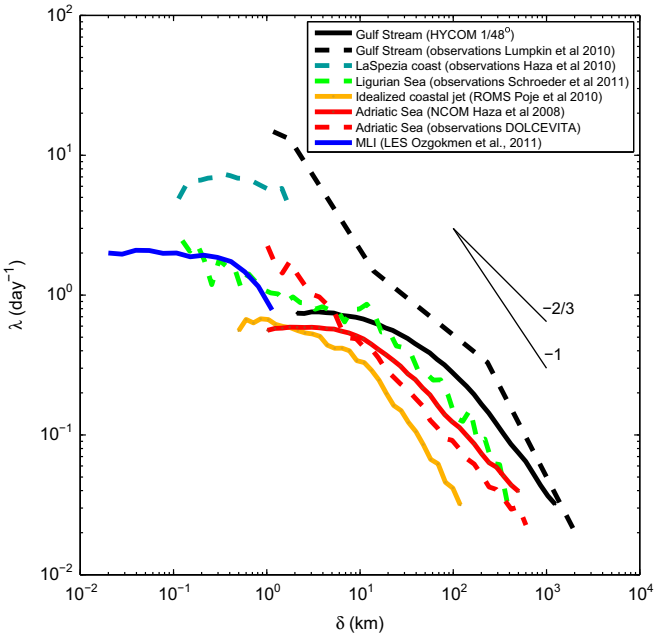

Fig. 5. A compilation of scale-dependent FSLE curves from observations (dashed) and models (solid lines) in studies conducted mostly by the authors in recent years. Ballistic ($\lambda \sim \delta^{-1}$) and Richardson ($\lambda \sim \delta^{-2/3}$) regimes are indicated.

2008; Thomas et al., 2008), which in turn influences the dynamics of transport. Another possibility is topographic effects in coastal regions. Finally, wind forcing is almost certainly important for near-surface measurements. Nevertheless, these factors are far from being sorted out yet on the basis of existing few studies.

Overall, the impact of multi-scale interactions on transport is a very exciting future research to pursue, and certainly, additional studies are necessary especially involving direct measurements of the ocean. This issue has a number of very relevant practical consequences. If transport is indeed dominated by mesoscale features, then state of the art eddy-resolving operational models can be used to describe transport pathways, possibly complementing them with Lagrangian data assimilation to improve mesoscale feature description and using dynamical system methods to locate LCS. This is the best scenario we can hope for in terms of transport predictability, and the results presented in this paper tend to support its feasibility. On the other hand, if submesoscale processes influence transport at various scales, then transport predictability could be very hard to achieve given the present limitations on model resolution and data assimilation coverage. Another possibility is that submesoscales processes are intermittent. These various scenarios and possible implementations are under active investigation at the moment.

4. Improving model velocity and transport using Lagrangian data assimilation

The results in Section 2 provide positive indications on the feasibility of identifying the main transport pathways from known velocity fields. In particular the results on the Gargano Cape in the Adriatic Sea show that model outputs, at least in some conditions, can be used to successfully compute the HTs and the LCSs of the flow. This positive result, though, cannot be generalized to all flows and model results. The circulation in the Adriatic Sea is strongly influenced by topography, so that the position of the HT is likely to be linked to topographic features and to be semi-permanent, as suggested also by fact that its signature is present in the pattern of historical drifters (Veneziani et al., 2007). The time dependence of the HT, at least at the surface, is likely to be mostly linked to the wind and to its associated Ekman transport, which are often correctly reproduced by the models. In other situations, for instance in open ocean regions without strong topographic constraints, we can expect that it could be much more challenging for models to correctly capture the positions of HTs and LCSs. The main structures such as vortices and jets are usually reproduced by the models, but their exact position might not be correctly identified, influencing the pathways of transport. A common problem with models, for instance, is related to the propagation velocity of the structures, so that there might be phase shift errors involving the exact location of the structures at a given time. As a consequence, relying solely on model results to compute transport pathways can be problematic at times.

A very effective avenue to improve model performance is to use real-time data to correct their results using methods of data assimilation. In particular, in our case, since we are interested in transport, we can expect that Lagrangian data from floating instruments that directly sample current advection will be especially useful. As discussed in Section 1, a number of different assimilation methods have been presented in the literature. Here we focus on a method, Lagragian in nature, that has been developed by the authors and other collaborators and that has been used and tested with in situ-data in a number of recent applications.

The method is based on a variational approach (Lagrangian Variational Analysis, LAVA, Taillandier et al., 2006a), and its practical implementation can be summarized as follows. The first and most crucial step consists in correcting the model velocity field at the level where the instruments are transported by the currents (i.e. at the surface for drifters and in the interior ocean for Argo floats), by requiring minimization of the distance between observed positions and positions of numerical trajectories launched in the model (Molcard et al., 2003; Taillandier et al., 2006a). The local correction along the trajectory is assumed to be characterized by some basic correlation scales in time and space that characterize the Eulerian persistence of the flow. The correction is performed over time sequences that are required to be shorter than both the Eulerian and Lagrangian time scales (Molcard et al., 2003). Once the velocity is corrected at the level of the data, as a second step, the correction is statistically projected in the water column using results from data if available or otherwise from the model itself. Finally, the other variables of the model, i.e. the water mass properties (temperature T and salinity S) and the sea surface height (SSH), are adjusted using some simplified dynamical requirements such as geostrophy and mass conservation (Özgökmen et al., 2003).

The method has been first thoroughly tested using the twin experiment approach in models of increasing realism (Taillandier and Griffa, 2006), and then applied to the assimilation of Argo floats (Taillandier et al., 2006b) in the Mediterranen Sea as part of the MFS (Mediterranean Forecasting System) project. Mediterranean Argo floats (MedArgo, Poulain et al., 2008) are programmed to drift at a parking depth of 350 m, resurfacing at approximately 5 day intervals, and providing information on their position and on T and S profiles. Lagrangian assimilation uses the position information to correct the drift at 350 m, and then projects the correction in the vertical and it adjusts the mass state variables assuming an approximate geostrophic balance. The results show a significant and consistent modification of the velocity field and of the mass variables, and the method has been transitioned to the operative MFS system (Taillandier et al., 2010).

Further investigations have been performed using surface drifter data. Assimilation of surface drifters is expected to be more challenging than for Argo floats mostly because they sample the very surface of the ocean (from 15 to 1 m), that is characterized by small scales fluctuations and dynamics that significantly deviate from geostrophy. This poses two significant question. The first one is related to which scales should be filtered and which ones retained in the model correction, while the second one is related to the correction of the mass variables, that has to be performed differently than in the case of Argo floats. A simple geostrophic balance in fact cannot be used since the upper meters are strongly influenced by Ekman dynamics and possibly also by ageostrophic submesoscale dynamics, so that a more complex decomposition has to be adopted. So far, we have been working only on the first step of assimilation, i.e. on the velocity reconstruction at the surface using drifter data. For the purpose of the present paper, reconstruction of the velocity is actually the most relevant step from the point of view of improving the identification of transport pathways, and it is discussed in details in the following.

Two main applications have been performed. The first one considers surface reconstruction in the Adriatic Sea using drifters in the upper 1 m and outputs of the ROMS model (Taillandier et al., 2008). The analysis focuses mostly on the impact of the velocity correction on the exchange between the boundary current and the interior. The results are qualitatively consistent with indications from satellite data, but a true quantification using independent data is lacking. The issue of independent data testing has been addressed in a more recent application in the Pacific Sea off Taiwan (Chang et al., 2011), where data from 30 Surface Velocity Programme (SVP) drifters drogued at 15 m and 28 sonobuoys with instrument chains were used in the framework of an operational exercise (LWAD07), together with the outputs of an NRL (Naval Research Laboratory) data assimilating model EAS-16 (East Asian Seas).

The LWAD07 region is especially challenging since the launching area was small (approximately 1/2 degree square) and situated at the edge of the Kuroshio Current. Both drifter and sonobuoy data sets (Fig. 6A,B) show the presence of two distinct regimes occurring in the restricted domain, separated by a sharp transition area. The western side is characterized by shelf dynamics with a significant tidal component, while the more eastern part is dominated by the highly energetic meandering of the Kuroshio current. The drifter and sonobuoy data sets, even though qualitatively similar, have significant quantitative differences, with the sonobuoy trajectories being overall slower and with slightly different orientations than the drifters. This is likely to be due to the fact that sonobuoys respond to currents at different depths, and also they have been launched in slightly different points and times with respect to the drifters. The EAS-16 model does not capture the presence of the two regimes, and its synthetic trajectories (Fig. 6C) show a more homogeneous northeastward motion with a strong tidal component. This is not surprising, given the high nonlinearity of the flow that makes

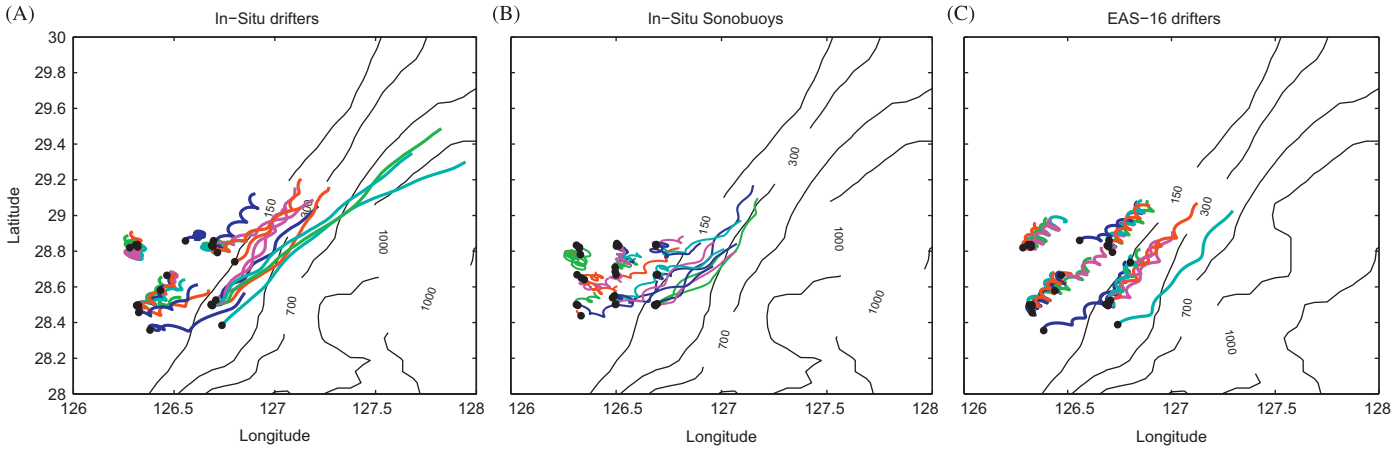

Fig. 6. (A) Observed drifter trajectories (B) observed sonobuoy trajectories and (C) modeled drifter trajectories in the LWAD07 region off Taiwan using EAS-16 during the first two days of the experiment, October 8–10 2007. Adapted from Chang et al. (2011).

difficult to predict its detailed structure, and the small size of the target area with respect to the resolution of the assimilation observing system.

The velocity fields of the EAS-16 model are corrected using the data from the drifters, and the corrections are statistically propagated from the drifter depth to the water column using the statistics of the (uncorrected) EAS-16 fields. An example of the velocity field and its correction at the drifter level is shown in Fig. 7. The drifter data tend to widen the extension of the Kuroshio meander, increasing the velocity in the eastern side of the sampled area (around 28.5° lat and 126.8° long), while they tend to decrease the velocity on the shelf area. The net result is a clear sharpening of the front in the region of interest. A first test, primarily of self consistency, is performed comparing the synthetic drifter trajectories computed with and without the correction with the observed ones. As expected the drifter trajectories from the corrected model are quite similar to the observed ones and they show the significant difference between the two regimes. At the quantitative level, the error is decreased with a gain of approximately 75%.

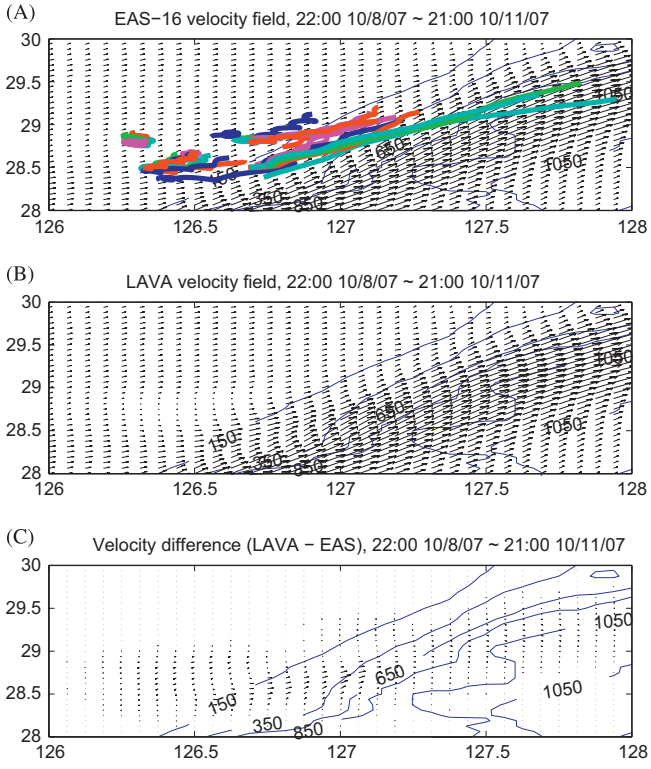

Fig. 7. Surface velocity vectors that show flow pattern in the LWAD07 region. The velocities are averaged over 3 days from 22:00 October 8 through 21:00 October 11, 2007. (A) original EAS-16 velocity; (B) corrected LAVA velocity; (C) velocity difference (LAVA - EAS-16). The zero velocity nodes are removed for easier reading. The trajectories of the drifters used in LAVA are superimposed on panel (A). Adapted from Chang et al. (2011).

A second and more significant test is performed using the independent data set provided by the sonobuoys. Synthetic sonobuoy trajectories are computed from the uncorrected and corrected velocity fields using an appropriate drift model (that describes the hydrodynamic response of sonobuoys in terms of distributed drag in the upper 27 m), and the synthetic trajectories are compared with the observed ones and with the ones computed from the EAS-16 without corrections. A visual example is shown in Fig. 8, clearly showing the improvement of the trajectories in the presence of correction. At the quantitative level, the error decreases less than for the drifters (as expected), but still significantly, with an error reduction of approximately 50%.

In Chang et al. (2011), an other method different from LAVA and developed by the University of Delaware has also been tested, that uses the velocities computed from the trajectories (instead of the positions) and is based on a normal mode decomposition (NMA, Toner et al., 2001). Both methods produce significant improvements, even though the NMA error reduction is smaller than the LAVA one (25% instead of 50% for the sonobuoy test). This is not surprising given that truly Lagrangian based methods, like LAVA, have been shown generally more effective (Molcard et al., 2003) when the time steps of correction are a sizable fraction of T_L as in this case. The fact that both methods provide significant advantages points out to the fact that the use of Lagrangian data to correct model velocities is indeed a powerful tool to improve trajectory and transport prediction.

4.1. Extended discussion and outlook

The results on velocity reconstruction using drifters summarized above point out to possible practical applications of the methodology for operational purposes using off line velocity outputs from models. Fast response strategies can be envisioned,

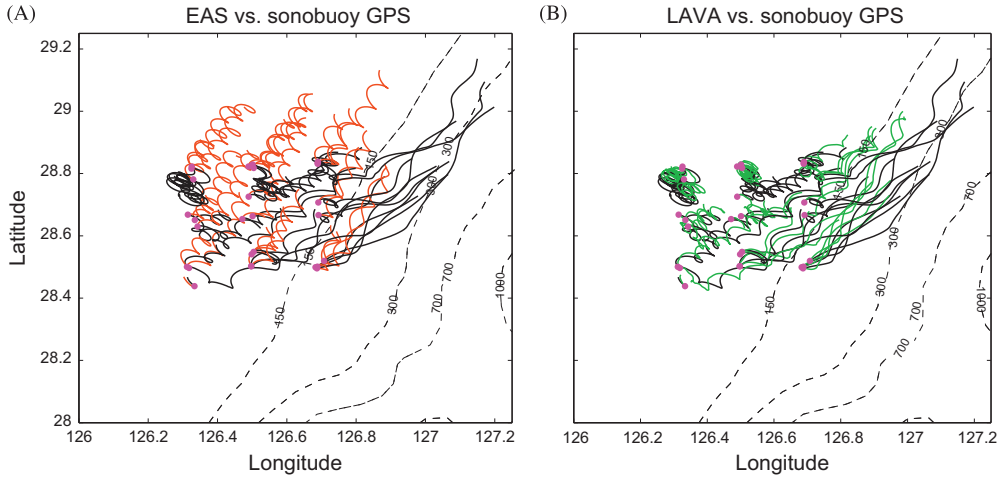

Fig. 8. Modeled sonobuoy trajectories in the LWAD07 region using the EAS-16 (red, A) and LAVA corrected (green, B) model velocity fields, compared to observed in-situ data (black) for two days after deployment. Adapted from Chang et al. (2011). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

where in case of accidents at sea or pollutant dispersals, ad hoc drifter releases are performed and drifter information are blended with available model results to obtain optimized patterns of transport. This approach has the great advantage of high flexibility, since it can be implemented using any operational model output available at a given time in a certain area, but it lacks in long term predictability since it is not truly assimilating the information in the model. The trade off between flexibility and extended prediction should be evaluated depending on the specific applications.

Regarding the challenges for full assimilation of surface drifters, different approaches can be envisioned. In the framework of the variational methods discussed here, an increased knowledge of surface dynamics would be greatly beneficial and it could lead to an improved observational operator. An other alternative approach is to incorporate these complex dynamics implicitly in a forecasting system that computes the correlations as they evolve, for instance from an ensemble analysis.

All the works discussed so far deal with the assimilation of data from Lagrangian instruments. A parallel and in some ways complementary approach includes the assimilation of tracer data observed from satellites, as tracer evolution is linked to flow advection. There are of course some constraints in the use of tracers as "Lagrangian" information, since the evolution of tracers such as SST and chlorophyll concentration is strongly influenced by their own dynamics or "fate", including external sources and sinks. Nevertheless, especially in the open ocean away from the influence of boundaries and for appropriate time windows, tracers data can provide valuable information. Tracer assimilation has been developed along two main lines. The first one corrects the velocity field using information from sequential tracer images, i.e. taking into account tracer evolution and linking it to advection processes (Horn and Schunck, 1981; Mercatini et al., 2010; Herlin et al., 2004). The second approach instead directly uses tracer image data (Direct Image Assimilation, DIA) extracting information from their pattern (Titaud et al., 2010).

Of particular interest here is a recent paper where DIA techniques are used to assimilate tracer using sophisticated observational operators based on FTLE or on the related Finite Time Lyapunov Vectors (FTLV) (Titaud et al., 2011). Conceptually, the method is based on the underlined assumption that high resolution information on tracer patterns showing submesoscale fronts and filaments are linked to chaotic advection induced by mesoscale features (Beron Vera et al., 2010). This implies that a correspondence is expected between the high resolution patterns of tracers and the Lagrangian patterns computed from local Lyapunov extrema from low resolution models. A simple method is used for pattern extraction from the images, based on the binarization of gradient norm using a hard threshold, and a cost function is established that minimizes the distance between tracer and FTLE or FTLV patterns. The authors show in the framework of an idealized twin experiment that the cost function is sensitive to variations of the model velocity and it has a well defined minimum. The approach is interesting, even though it needs further testing for real ocean applications also in terms of range of validity of the basic assumptions linking tracers and LCSs.

5. Remarks and open questions

The methodologies discussed in the previous sections can be considered complementary in many respects. Dynamical system theory focuses on identifying the main transport pathways in a given flow, by locating distinguished finite-time invariant boundaries in the Lagrangian frame. The approach is fully deterministic; it relies on the assumption of a correct knowledge of the Eulerian flow, which is often not completely the case for the velocities reproduced by the models. Lagrangian data assimilation (or reconstruction), on the other hand, aims at improving the model velocity and transport by taking into account information from data provided by floating buoys. The methods are different from the technical point of view, as they use different mathematical tools, but they have in common the same basic conceptual approach. The methods in fact share the Lagrangian approach, namely the idea that the velocity field and its associated transport are best described in a Lagrangian frame. This is exemplified for instance by the fact that targeting Lagrangian structures in data assimilation can lead to optimization of data sets (Poje et al., 2002). Hyperbolic trajectories HTs, that are identified by dynamical system theory as the crucial points regulating transport, also play an important role in Lagrangian data assimilation, since trajectories launched around the HT provide optimal sampling (Molcard et al., 2006), correcting the velocity field in the most effective way with respect to other launching schemes such as homogeneous coverage or coverage of other regions of the flow. On the other hand, it should also be noted that the nonlinearity of HTs can challenge some assimilation schemes (Kuznetsov et al., 2003; Salman et al., 2006), leading to divergence in Kalman Filtering or Extended Kalman Filtering which can be removed using a particle filtering approach (Spiller et al., 2008). Also, it should be noted that the sampling in the HT region has to be appropriate. Information from a single trajectory, for instance, could fail to appropriately convey the presence of an HT and therefore the correction could be misleading. Different is the case for elliptic points, that can be characterized even by a single trajectory (Veneziani et al., 2005a), allowing for a successful assimilation of the structure. In other words, while HTs are indeed the points with higher potential information, they have to be treated appropriately to actually retrieve the information correctly.

The two methodologies, i.e. dynamical system theory and Lagrangian data assimilation, have also in common some basic assumptions and limitations. The main assumption is that transport is mainly regulated by mesoscale structures. This is implicit in the methods to compute LCS as well as in the implementation of Lagrangian data assimilation which typically assumes that the Eulerian time scale T_E of the structures is significantly longer than the Lagrangian time scale T_L. In the last few years, a growing attention has been devoted to the existence and role of submesoscale motions characterized by scales of the order of few km and few days or less. Theoretical and numerical works at high resolution (Capet et al., 2008a, 2008b) suggest the emergence of these motions in the surface ocean, triggered by processes of stirring frontogenesis and ageostrophic instabilities. They are expected to play an important role in the processes of energy cascade in the ocean and in vertical transport and bio-geochemical fluxes. The actual geographical distribution of submesoscale processes in the ocean and their influence are still unknown (Griffa et al., 2008; Munk et al., 2000; Rudnick, 2001), since experimental results are still limited due to the high resolution requirements and to the occurrence of space-time aliasing in measurements at those scales.

Another basic assumption in common between dynamical system theory and Lagrangian data assimilation is the fact that ocean structures are considered primarily two-dimensional (2-D). The majority of ocean LCS studies so far have been restricted to time-varying flows that are spatially 2-D, while Lagrangian data assimilation (and reconstruction) primarily focuses on the correction of the velocity field at a given depth, eventually projecting the correction in the vertical. Clearly, the 3-D nature of ocean structures can have an important role in transport pathways at various scales. Not only submesoscale features are expected to be associated to significant vertical transport, but also mesoscale

eddies are influenced by 3-D fluxes of mass, buoyancy and momentum.

A possible avenue for a more complete 3-D Lagrangian description is to use additional information on the water column, for instance from natural and experimental tracers. An example is given in Fig. 9 in the context of tracer release in a large eddy simulation (LES) of mixed layer instability (MLI), described by detail in Özgökmen et al. (2011). MLI is a form of baroclinic instability that tends to take place in frontal regions of surface mixed layers, and it is a relatively new and so far not well-observed paradigm put forward as an important process in mixed layer adjustment and restratification (Boccaletti et al., 2007). In Fig. 9 upper panel, the tracer is initialized with a value of 0 in the upper 50 m and 1 elsewhere, resembling nutrient distribution in the ocean. The resulting upwelling patterns at the surface (Fig. 9 middle panel), consisting of thin elongated filaments and resembling submesoscale features seen in satellite images (http://oceancolor.gsfc.nasa.gov/cgi/image_archive.cgi?c=CHLOROPHYLL), are qualitatively consistent with frontogenetic dynamics associated with horizontal stirring processes suggested on the basis of simplified (surface quasi geostrophic, SQG) dynamics (Klein and Lapeyre, 2009). Nevertheless, a detailed look at the 3-D tracer distribution indicates a very complex stretching and folding of the tracer field while undergoing upwelling along the isopycnal representative of the MLI (Fig. 9 lower panel).

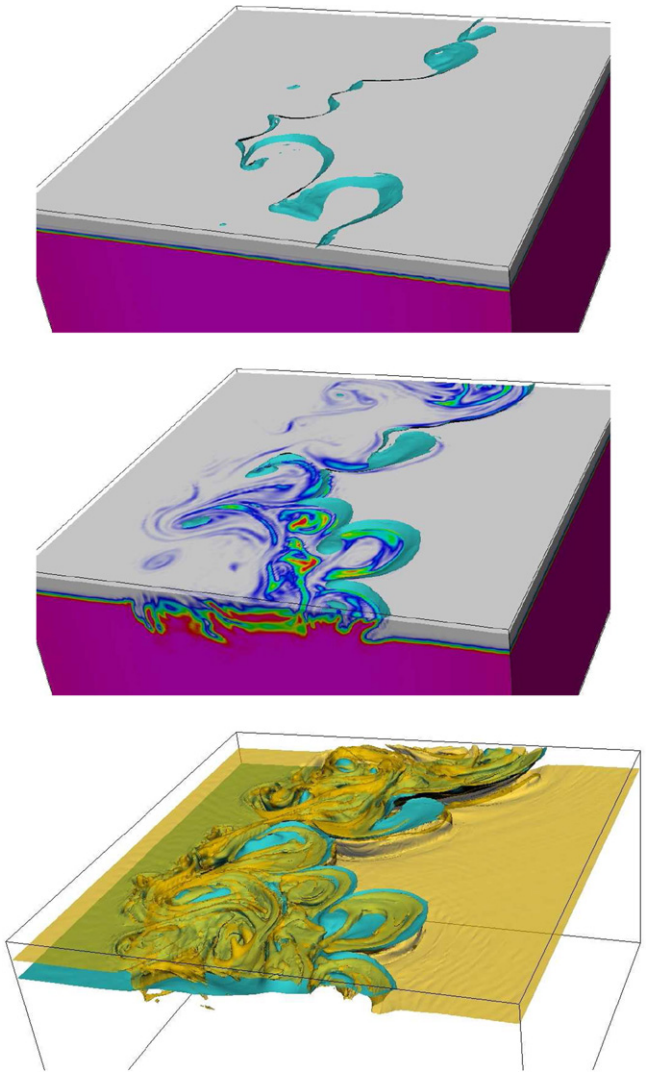

Fig. 9. (Upper panel) Tracer initialization with concentration of 0 (gray color) in the upper 50 m and 1 (magenta) in the rest of the domain in a LES of well-developed mixed layer instability described in Özgökmen et al. (2011). Representative isopycnal surface of the mixed layer instability is shown in turkquoise color. The domain is 10 km × 10 km × 0.5 km in the x, y and z directions, respectively. (Middle panel) Surface signature of the tracer concentration after 5 days of integration, indicating that upwelling along mixed layer isopycnals has taken place. (Lower panel) 3D, complex distribution of the tracer interface after 5 days. See also: http://www.rsmas.miami.edu/personal/tamay/3D/mli108-tr-v2.mov and http://www.rsmas.miami.edu/personal/tamay/3D/mli108-tr-v1.mov. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

Further progress in the understanding of such 3-D Lagrangian dynamics in the ocean relies on developments in theory, observations and modeling. Regarding theory on dynamical system methods, different approaches have been proposed. Branicki and Kirwan (2010) have generalized the 2-D dynamical system approach by computing LCS at various depths of the flow, as horizontal slices embedded in a 3-D volume. This method, even though limited by the basic assumption that the flow is nearly nondivergent, has allowed some interesting diagnostics of vertical transport pathways. Emergence of new and fully 3-D LCS has been theoretically outlined by Mezic (2001). There is a new effort with the objective of exploring these ideas in idealized and realistic flows at different scales (http://www.whoi.edu/ocean3dplus1). In terms of observations, an exciting avenue is the development of airborne laser tracking method of near-surface (upper 30–50 m) tracers (Sundermeyer et al., 2007). Also, 3-D floats developed by D'Asaro (2003) constitute a very useful complement to tracer releases, since they provide position and velocity information as opposed to concentration, especially if much larger numbers would be available in the future. Finally, regarding modeling, LES studies provide fully 3-D dynamics and in most cases numerically very accurate results. LES approach relies on the solution of Boussinesq equations with no or minor degree of parameterizations, with the exception that complex surface effects, such as Langmuir cells, need to be explicitly parameterized (Skyllingstad and Denbo, 1995). We envision such models becoming a fundamental part of future 3-D Lagrangian studies.

6. Summary

In this paper, two different and complementary methods to improve our understanding of transport pathways in the ocean are discussed, namely methods from dynamical system theory and from Lagrangian data assimilation. Research in these two fields has been very active in the last decade, and many new techniques have been proposed. Results have been thoroughly tested in the framework of numerical models, but practical applications to real ocean flows including Lagrangian in-situ data testing are still limited. Here we provide a review of contributions given by the authors in terms of method implementations and applications to oceanographic flows and data, discussing them in the general framework of the extended results related to these methodology.

Two applications of dynamical system theory are presented, obtained in the framework of two experiments in the Mediterranean Sea. The first experiment took place in the Adriatic Sea in the Eastern Mediterranean, off the Gargano Cape, and it involves flows with typical mesoscale deformation radius of the order of 10 km. The second experiment instead involves a more coastal flow inside the Gulf of La Spezia in the Western Mediterranean, with deformation radius of the order of few km. In both cases, FSLEs have been used to compute LCS based on velocity fields, provided by an operational model in the Adriatic case and by VHF radars in the case of the Gulf of La Spezia. In both cases, the results are found to agree with independent data of drifters

launched in the areas. The drifter paths are consistent with the LCSs and do not cross the time-varying barriers indicated by the FSLE ridges.

A few conceptual points can be drawn from these results. The first one is that transport pathways can indeed be characterized by LCS in flows at different scales, from offshore to coastal flows, provided that there is a dominant mesoscale structure. The second point is that velocity fields from radars and models can be used as a basis to compute accurate LCS structures. One important question, though, is how general this last finding is. Radar data have been used also by other authors to compute LCS (Shadden et al., 2008) with similar positive results. Model based results, on the other hand, might be more dependent on specific applications. The Adriatic Sea is strongly topographically constrained, and the HT identified by the model might be linked to a topographic feature, with a time dependence mostly due to wind induced Ekman dynamics in the upper layer. This is a relatively simple situation for a model to reproduce, differently from what is expected to happen for instance in an open ocean flow without topographic constraints and dominated by strong nonlinearity. In this type of applications, models might not be able to correctly reproduce the exact position of the main ocean structures, and therefore methods like Lagrangian data assimilation might be especially valuable to correct the flow.

A case of this type is discussed here in the framework of the review of results for Lagrangian data assimilation obtained by the authors using a variational approach (LAVA). The application is performed in the Pacific Ocean off Tawaian with data taken in the framework of an operational exercise LWAD07. The region of interest is quite challenging, since it consists of a relatively small area at the boundary between the meandering Kuroshio Current and the more quiescent shelf area. The 30 drifters launched during LWAD07 show two distinct regimes in the area separated by the Kuroshio front. The operational model outputs do not correctly reproduce the exact frontal position, so that the synthetic trajectories are distinctively different from the in-situ ones, showing an homogeneous drift. The model fields have been corrected using drifter data and the correction has been propagated in the vertical. Results have been tested quantitatively using trajectories from sonobuoys, i.e. floats with instrument chains. The positive results, showing an error reduction of 50%, indicate the high potential of Lagrangian data assimilation. It should be noted though that LAVA is applied here only to the velocity reconstruction rather than full assimilation (as for the Argo floats applications in the interior ocean, Taillandier et al., 2006b). Full assimilation implies that also the mass variables are corrected, using for instance some simplified balances such as geostrophy. This is acceptable in the interior flow, but in the upper ocean the dynamics are not well known and they are likely to have strong ageostrophic components. A possible approach to be used in future works could be to implicitly incorporate this complex dynamic information in a forecasting system that compute the correlation evolution in time for instance from an ensemble system.

While the paper is specifically concerned with methods and applications dealing with Lagrangian data, we have also discussed the links with other results dealing with information on tracer fields from satellite. Tracer patterns, at least in the open ocean and under some restrictions, provide information about time integrated transport and are therefore been used to validate the presence of LCS in the ocean. They have also been used in various capacities for assimilation in numerical model in order to correct the velocity field. In a recent paper, an observational operator including LCS descriptors have been proposed for tracer image assimilation (Titaud et al., 2011). The differences between satellite tracer data and in-situ Lagrangian data with respect to information content, techniques and outlook have been discussed.

A critical discussion of the two general approaches is provided, indicating their common assumptions and their present limitations. Both approaches assume that transport is primarily controlled by mesoscale features, and that it is primarily 2-D. These assumptions are presently under investigation. Recent works show that submesoscale processes are likely to be relevant in many surface ocean flows in terms of energy cascade and vertical transport. Their role in horizontal transport and their influence on mesoscale pathways are still not clear. The results discussed here suggest that mesoscale is indeed dominant in transport and dispersion, but other results on relative dispersion from data and models provide a quite complex picture that still need to be unravelled. There might not be a generic answer to this question, and the relevance of submesoscale might be dependent on region dynamics. Even in regions where submesoscales are relevant, they might influence transport only locally, i.e. at their own scales. If this is the case, a possible avenue to take them into account is to parameterize their action, while maintaining eddy resolving models as a basis for computing mesoscale transport. Finally, possible avenues on transition to 3-D Lagrangian analysis are discussed.

Acknowledgments

The authors thank Tom Rossby for numerous inspirational discussions occurred during the years, that have deeply influenced their work. The authors also acknowledge discussions and exchanges with Andrew Poje, Denny Kirwan, Leonid Piterbarg, Enrico Zambianchi and Michel Rixen. We greatly acknowledge the support of Office of Naval Research under Grants N000140510094, N000140510095 and N000141110087 and the National Science Foundation under Grant OCE-06040000.

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