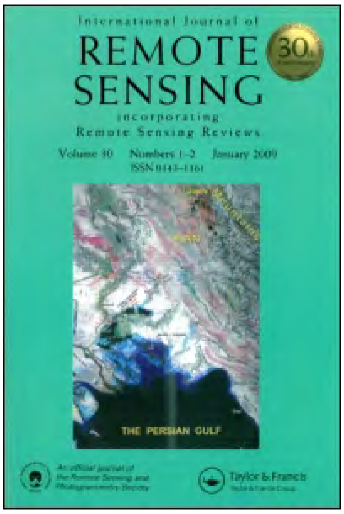

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Extending the use and interpretation of ocean satellite data using Lagrangian modelling

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We propose a new methodology for synthesizing satellite or *in situ* observations with ocean circulation velocity fields from an operational model. This is done by attaching values taken from the satellite observations to virtual particles seeded at the surface in the domain of a circulation model and advecting them in a Lagrangian fashion. It is then possible to track the fate and change in composition of individual water parcels between two satellite images, and hence estimate the change in satellite-derived properties along the trajectories of water parcels. The power of the method lies in deciphering the change in sea surface properties from satellite data in the Lagrangian (advective) frame. We use this to estimate rates of biological processes. Further, we generate a dynamically correct time-interpolation of satellite fields by considering the temporal change in water properties as occurring along trajectories of moving water parcels, rather than in a static medium. We use the methodology to interpret and interpolate MODIS satellite fields in the Gulf of Maine, which has notoriously intermittent satellite coverage. The dynamic interpretation is made possible for this region by the availability of time-specific velocity fields from an operational coastal circulation model.

1. Introduction

With repeat coverage, high spatial resolution and improving radiometric sensitivity, satellites have revolutionized the way in which surface processes on land and ocean are studied. The MODIS sensors on the NASA Aqua and Terra platforms capture a range of visible and infrared (IR) data suitable for the study of land, ocean and atmosphere. Its suite of ocean colour data, typically processed at 1 km spatial resolution, are used to produce a variety of biophysical products including sea surface temperature (SST), phytoplankton pigment, coloured dissolved organic matter, spectral absorption, backscatter, and attenuation depth (MODIS Algorithm Theoretical Basis Documents, NASA).

Currently available satellite ocean products, however, have major shortcomings when it comes to interpreting the time evolution of biophysical processes. Firstly, clouds obscure the satellite instruments' view and leave many a satellite pass with partial or zero coverage of a region. Thus, temporal information at any given location is intermittent. Secondly, the change in a surface ocean property observed at

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any location is due to (a) the advection of the property with the circulation, and (b) the change in the satellite-derived value attributable to biogeochemical processes. The advective contribution to the change is often sizable or larger than the change due to growth/decay. In the case of biological properties derived from ocean colour data, the time scales for advection T_a ($T_a=L/U$; for length scales $L=10$–100 km and velocity $U\sim0.1\,\mathrm{m\,s}-1$), and biological growth T_b, are of similar magnitude and typically 1–10 days at the scales of observation. Hence, it is difficult to decipher the rate of change in properties in the moving medium or directly compare satellite images from different times to assess the change that the properties are undergoing.

The use and interpretation of satellite fields could be extended if studied within the moving frame of the ocean's circulation. In such a Lagrangian view, one should imagine processes acting within a moving water parcel, so that any observed change in property is then due to growth/decay, or sources/sinks, and not contributed by advection. In the case of biological fields, the growth/decay can be translated into a productivity rate, which is of interest for understanding biological efficiency and carbon cycling. For example, the change in the organic carbon stock over the euphotic layer reflects the net rate of fixation of inorganic carbon, and can provide information about the strength of the biological carbon pump.

In the methods we propose for interpreting satellite data, we integrate the satellite fields with ocean model circulation fields to cast them in the moving frame of the circulation. This is done by assigning satellite-derived property values to neutrally buoyant particles seeded uniformly in the surface layer within the domain of an operational circulation model, and advecting these with time-dependent velocity fields from the model until the time that the next satellite observation is available. The change between the previously assigned satellite value and the newly available satellite value, divided by the time between observations, is the (Lagrangian) rate of change in property along the water parcel's trajectory. This Lagrangian rate of change is within the advective reference frame and is the growth/decay (or source/sink) rate, which is of interest in physical and biological process studies.

The tremendous growth of operational ocean modelling, particularly in coastal regions, offers the opportunity of combining ocean velocity fields with satellite data to enhance the applicability and interpretation of both. Although modelled velocity fields are not without error, our experience shows that using an operational model with high fidelity to drive a large number of virtual particles produces a useful basis for the interpretation of satellite fields. Several important applications can be developed from the methodology. Firstly, it enables us to estimate the growth/decay rate of satellite-derived properties, including a synoptic, time-evolving view of ocean productivity. Secondly, it allows interpolating satellite data along water parcel trajectories. Such a Lagrangian interpolation captures the dynamic quality of the ocean and has many advantages over other satellite interpolation methods, that do not account for such motion. Thirdly, the Lagrangian trajectories can be used to trace water masses with different characteristics. This could be useful for tracking river plumes and the constituents of terrestrial runoff or for identifying biogeochemical property relationships that are specific to a water mass or source of runoff.

In what follows, we describe our modelling methodology and then apply it to satellite data and circulation model fields in the Gulf of Maine. We then present some results from the applications described above. We include a discussion of model error, limitations of the method for the application, and improvements that could follow.

2. Methods

The Lagrangian methodology we describe is applicable to any ocean surface property that is measured repeatedly and thus, is amenable for use with any satellite-derived product. It can be used with any reliable model velocity fields, or with surface velocity data obtainable from high frequency radar networks. Here, we describe a study that applies the methodology to enhance the interpretation of satellite ocean colour data in the Gulf of Maine. The underlying motivation for this work is to improve our understanding of biological productivity and oceanic carbon cycling on the continental shelf.

2.1 *Satellite data*

Quality controlled, level 2 ocean colour products processed from MODIS Aqua and Terra platforms are served by the University of New Hampshire's Center of Excellence for Coastal Ocean Observing and Analysis for the Gulf of Maine and surrounding regions. Typically, in this region, the satellite produces two images in the afternoon; the earlier is preferred for a better viewing angle. To gain a Lagrangian rendition of the MODIS ocean colour data in the Gulf of Maine, we parse through an archive of satellite images for the region. We select image pairs 2 to 6 days apart, a time interval that allows us to resolve temporal changes in the spatial patterns of relevant biological fields such as Chl_a. Increasing the time interval between satellite images has the disadvantage that it requires longer calculation of the Lagrangian trajectories, thus admitting greater error in the trajectory paths and the diagnosis of growth/decay. In a given year, we find about a hundred such image pairs with a minimum spatial coverage of 30%. The method demonstrated here on one such an image pair can be repeated sequentially in time to generate a spatio-temporally evolving analysis/interpretation of a satellite product.

2.2 *Circulation model*

We perform the Lagrangian modelling with instantaneous velocity fields from an operational ocean circulation model (Xue *et al.* 2000) run at the University of Maine. The model, which derives from the Princeton Ocean Model (POM) (Blumberg and Mellor 1987), is set up and maintained through the Gulf of Maine Ocean Observing System (Go-MOOS). It is nested within a larger scale circulation model providing boundary conditions, is forced by operational winds and tides, and assimilates satellite SST and buoy data. Details of the model and validation studies against observations are described in Xue *et al.* (2000, 2005). We obtain the model horizontal velocity fields saved at 3 hourly intervals on an approximate $3.5\,\text{km} \times 3.5\,\text{km}$ curvilinear grid for the entire period from 2002 to present. Our model domain is chosen to be a subregion of the Gulf of Maine model and consists of 164×80 grid cells.

Though the circulation model is three-dimensional, we restrict ourselves to using only surface velocities for the interpretation of the satellite fields. At 10–100 km scales in the ocean, flows are largely two-dimensional and the vertical velocity component is smaller than the horizontal components by three or four orders of magnitude. The vertical velocity field in most numerical models is therefore highly sensitive to changes in resolution, forcing, and small perturbations. Even so, changes in a surface property's signature due to vertical motion will be seen in the satellite data and recorded by this method.

2.3 *Lagrangian modelling*

We use the Lagrangian particle tracking model (de Vries and Doos 2001) to advect particles within the model domain. The model grid is seeded evenly with 50 particles in each cell. Particles are advected from the time of the first to the second satellite image of each image-pair using time-dependent velocity fields interpolated in space and time on to the sub-grid positions of the particles. The advection trajectories of particles are computed from a path integral that is not restricted to the resolution of the grid. Though our Lagrangian tracking module is three-dimensional, we tie the particles to the surface for the interpretation of satellite data.

At the time of seeding, the particles are assigned concentrations (e.g. satellite-derived Chl_a) from the first of two sequential satellite images. Next, the particles are advected forward in time using the relevant time-specific surface velocity fields until the time that the subsequent satellite image is available (within the span of 2–5 days). Finally, at this time, the new satellite values at the newly assumed positions of particles are read in. Had there been no change in the chlorophyll due to biological production (phytoplankton growth/decay), the value of Chl_a at the new locations and time would be the same as the values ascribed to the particles at the start of their trajectories. If we assume accurate modelled fields and satellite retrievals, the difference or change in value between starting and ending positions, is ascribed to growth/decay or biological production/consumption and changes in concentration due to vertical mixing, advection, and sinking. Hence our estimate of growth/decay incorporates, but does not distinguish, such processes.

In order to display the spatial distribution of Lagrangian property changes along a water parcel trajectory, we need to reference the property change to a location, i.e. to some point on the trajectory. In all the results presented here, we reference the Lagrangian change to the starting position of the trajectory. The trajectory modelling is done offline, i.e. using the velocity fields produced by the circulation model, but separate from it. This is computationally efficient and enables seeding the model-domain with several hundred thousand particles. Thus, even if individual trajectories are in error due to misdiagnosed velocities, we generate credible results based on the statistics of several hundred thousand particles.

The Lagrangian approach has several advantages when trying to combine velocity fields with satellite data. Most importantly, we can deal with uneven and sparse spatial distributions, for example when data is missing due to cloud cover. Particles are assigned concentrations as per the availability of data. They serve to diagnose a change in concentration (or to interpolate between two fields in time) when data is available at the start and end positions of the particle trajectories, but are advected in the circulation, irrespective of the satellite data. This has an advantage over using a tracer advection scheme, since patches with no data would create steep gradients and artificial anomalies in the concentration field if tracers were used. Furthermore, limited domains with open boundaries are not a problem in our method since particles are allowed to exit the domain. The particles need not have discrete positions coinciding with the grid, and are hence not constrained to the spatial resolution of the circulation model.

3. Results

We demonstrate the applicability of this method by diagnosing the rate of change of satellite-derived properties as presented in a dynamic interpolation of satellite fields in the Gulf of Maine. Of great concern is the fidelity of the Lagrangian trajectories that form the basis of our diagnosis and interpolation. Thus the results section begins with an evaluation of advective errors.

3.1 *Validity of the modelled Lagrangian trajectories*

Xue *et al.* (2005) presents several model-data comparisons of the circulation fields that we use for the interpretation of satellite data. Here, we assess the effect of errors in the computation of particle trajectories arising from imperfect velocity fields, the interpolation of model velocities in space and time, numerical integration of the trajectory path, and the omission of vertical velocity. A further assumption is that the satellite data is representative of the vertically integrated property value in the upper few meters of the ocean, and that horizontal velocities from the uppermost grid cell layer of the model are the advective velocities that act on the satellite-derived properties.

To evaluate the advective error in trajectories, we compare the changes in Chl_a vs. SST between the start and end positions of particle trajectories advected between two satellite images separated by 2–6 days. Our assumption here is that on this time-scale, sources and sinks for the biologically active Chl_a field will be much larger than those for SST, which behaves more conservatively over these time scales. If SST were a passive tracer, i.e. with no sources/sinks, one would expect no change between the start and end values of SST along-trajectory for perfectly accurate trajectories. Thus a scatterplot of the end value vs. the beginning value along all modelled trajectories, would describe a perfect line with a slope of 1 : 1. If we now assume that the SST behaves passively, scatter about the 1 : 1 line would be attributable to errors in the Lagrangian modelling.

In figure 1, we plot values of Chl_a and SST at the start vs. end positions for 10 000 trajectories (a randomly picked subset of 500.000 trajectories) computed between two satellite images separated by 5 days. Here we show only one instance, but similar plots can be constructed for every satellite-image pair. The scatter from the 1 : 1 line in these plots results from a combination of (a) sources/sinks that alter the property, and (b) advective error in the Lagrangian trajectories that cause the particles to be incorrectly positioned with respect to second satellite field. We see that the spread from the 1 : 1 line is greater in the case of Chl_a than SST, suggesting that biological sources/sinks are indeed larger (faster acting) than those for SST. We can view the scatter from the 1 : 1 line for SST to be an upper-bound on the advective error, since it represents the sources/sinks plus advective error. Since the advective error is the same in both cases, this result provides assurance that model advective errors are, in general, a much smaller contributor to the total spread in figure 1(*a*), than the Chl_a source/sink being identified by the method. The histograms in figure 1(*b*) show the angular deviation of individual points on the scatter plots from the *x*-axis, with 0.785 radians denoting the 1 : 1 line. Points to the right of 0.785 represent trajectories along which the value of Chl_a or SST has increased, whereas points to the left denote decrease. The spread in SST is only a small fraction of the spread in Chl_a, which gives us confidence in ascribing the deviation in Chl_a to growth/consumption of phytoplankton. If individual trajectories have error, the statistics obtained from hundreds of thousands of advected particles are informative, and the histogram's median is likely indicative of the median rate of change of Chl_a for the region over which the trajectories are computed.

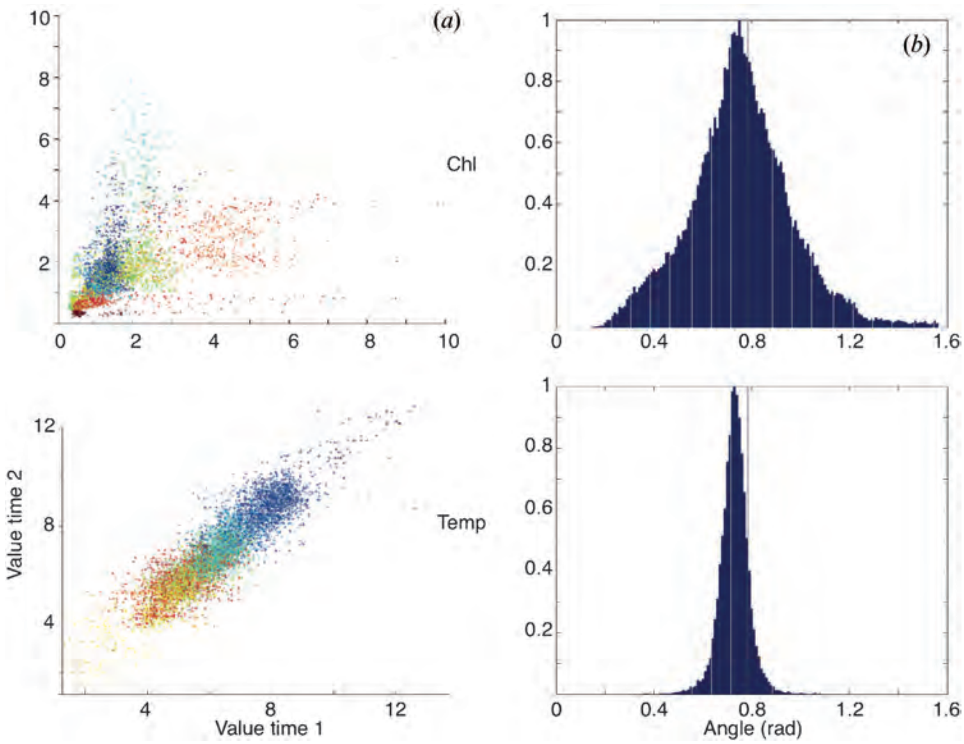

Figure 1. Sea surface chlorophyll (Chl_a), top row, and temperature (SST), lower row, from satellite are interpolated onto particle trajectories computed from the model surface velocities. The scatter plots (*a*) show the value of Chl_a and SST at the starting position, plotted against the value at the end position of each trajectory. The start and end times of the trajectories coincide with the first and second image from a satellite image pair separated by 2–6 days. Only a random subset of the several hundred thousand particles is shown. The colours in the scatter plots indicate distance from land with blue being far and red close. On the right (*b*), is the probability density function (pdf) of the angle made by each point on the scatter plot with the *x*-axis.

3.2 *Estimating property growth/decay*

To examine the change in property along Lagrangian trajectories, we consider the set of particle trajectories for which satellite data is available at the start and end position, which coincide with satellite observations from an image pair with at least 60% coverage, separated by 2–6 days. For each viable trajectory, we calculate the change in property divided by the time between satellite images to obtain the rate of growth/decay. This is plotted at the start location of each trajectory. For the purposes of displaying the result on the model grid, we average the value over all particles originating in the same grid cell.

Two subsequent satellite-derived distributions of a property (Chl_a, in this example) are shown in figure 2(*a*) and (*b*). The difference between these images, obtained by merely subtracting the second from the first, shown in figure 2(*c*), is due to sources/sinks, as well as changes caused by the advection of different water properties. By tracing Lagrangian trajectories, we are able to separate these two components and discern the sources/sinks, which are of interest in diagnosing productivity or growth. In figure 2(*e*), we plot the difference between the start and

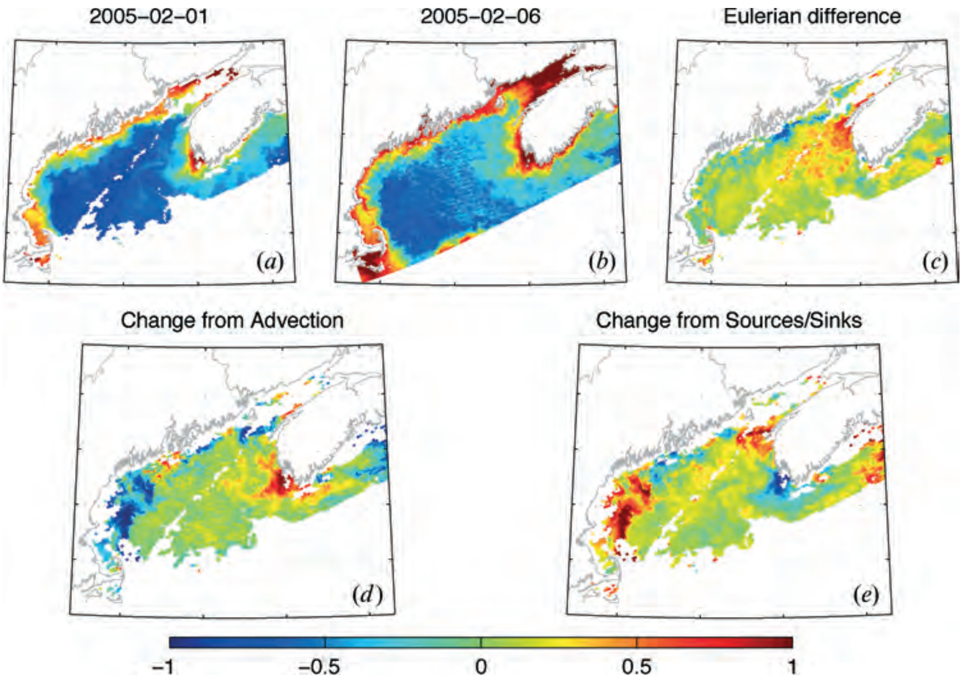

Figure 2. Panels (*a*) and (*b*) represent the Chl_a field in two satellite images of the Gulf of Maine from 2005-01-01, and 2005-01-06. Panel (*c*) is the difference calculated by subtracting panel (*a*) from panel (*b*). Panel (*d*) represents the advective component of the total difference, and panel (*e*) the change due to production and consumption of Chl_a. The change due to advection, shown in (*d*), is the part of the Eulerian difference in (*c*) that remains after the source/sink shown in (*e*) is subtracted. Calculation of panels (*d*) and (*e*) is based on Lagrangian tracking of water parcels.

end values of Chl_a along trajectories computed for the time between the satellite image pair. The start positions of trajectories, which were on a uniform grid, derive their satellite Chl_a value from the first image (*a*), whereas the end positions of trajectories derived their values from the second image (*b*), 6 days later. The along-trajectory difference, plotted in (*e*) at the start positions of the trajectories, represents the Lagrangian change, which is due to sources/sinks of Chl_a. To demonstrate the contribution of advection, we plot (in (*d*)) the difference between (*c*) and (*e*), which is the advective contribution to the Eulerian change shown in (c). We find that the advective contribution in (*d*) is comparable in size to contribution from sources/sinks in (*e*). This indicates that advection must be accounted on space- and time-scales such as these.

Contrasting the Lagrangian growth of Chl_a in (*e*) with the Eulerian change in (*c*), we find differences in the spatial distribution and sign of change in many locations. Positive values in the Lagrangian sources/sinks denote an increase of Chl_a along trajectories leaving that site, while negative values denote loss. The patch of positive values in the western Gulf of Maine indicate that water leaving this region acquired higher Chl_a as it moved away, in this case, to the south. Negative values south of the Scotian shelf denote that waters moving from here experienced a decline in Chl_a.

This Lagrangian growth/decay may be calculated for any satellite-derived property, and evaluating the growth/decay of various properties provides an

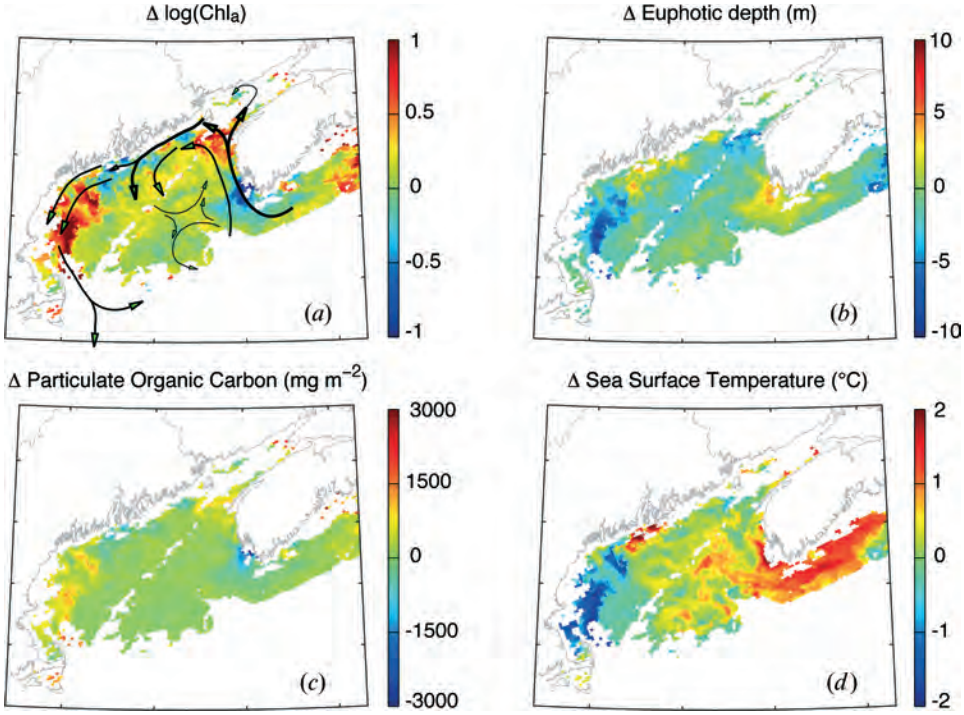

Figure 3. Changes in (*a*) Chl_a, (*b*) Euphotic depth derived from K490, (*c*) POC, and (*d*) SST, respectively, calculated using Lagrangian tracking of water parcels. Black arrows in panel (*a*) represent the general circulation in the Gulf of Maine, as described by, and adopted from, Pettigrew *et al.* (2005).

understanding of processes driving the changes. In figure 3, we compare the Lagrangian growth of Chl_a with that of the euphotic layer depth z_e calculated from the diffuse attenuation coefficient K_{490} as $z_e = \log_e(0.01)/K_{490}$, the particulate organic carbon (POC) content calculated as $POC = Chl_a\, z_e/\Theta$ where Θ is the Chl:C ratio and is approximated as 0.02. The growth of z_e is weakly anti-correlated with Chl_a, as increase in phytoplankton concentrations reduce the depth of light penetration. Along-trajectory changes in SST could occur by surface heating/cooling or by the upwelling and mixing of (cooler) subsurface waters. The latter case is generally associated with a supply of nutrients from subsurface to surface waters, and consequently a growth in phytoplankton and Chl_a. Thus, a correlation between the along-trajectory decline in temperature and increase in Chl_a as seen in the western Gulf, is indicative of vertical upwelling or mixing, while the increase in surface temperature in the eastern Gulf is indicative of warming.

While this method is able to account for the effects of vertical advection and mixing on the surface properties, we do not track the vertical motion of water parcels *per se*. The effect of upwelling is perceived through a change in SST or Chl_a. Similarly, a loss of phytoplankton by subduction or sinking would result in a decline in Chl_a and be accounted as a loss from the euphotic layer. However, it is difficult to discern between the loss of phytoplankton by sinking vs. that which would occur due to zooplankton grazing. Parameterizations for the sinking and mixing could be used to attempt to quantify the differences.

3.3 *Dynamic interpolation*

We can also use the calculated Lagrangian trajectories to interpolate satellite data over time, while accounting for the advection of features by the circulation. To accomplish this, we linearly interpolate a certain property along trajectories between the start and end values obtained from two satellite images. We average the Chl_a values of all particles positioned in a certain model grid-cell every 3 hours. The differences between a Lagrangian (dynamic) interpolation of Chl_a, and an Eulerian (static) interpolation of two fields can be substantial. An animation of such an example can be seen at http://niak.bu.edu/chl_anim.

The dynamic interpolation is able to account for the advection of features within the circulation field, while the Eulerian interpolation performs a static blending of two satellite fields. The difference in approaches can be noted in a Hovmöller diagram (figure 4) which shows the time evolution of Chl_a along a transect in the Gulf of Maine (figure 5 shows the location of the transect). The Lagrangian dynamic interpolation captures advective features and results in higher temporal variability in individual grid-cells than the conventional Eulerian method for interpolation. Figure 5 shows the temporal variance of Chl_a over time in each grid-cell. The largest difference in variability between the two methods occurs along the coast, where the large spatial variance in Chl_a is translated into temporal variance by advection.

This Lagrangian method aims to improve the coverage of satellite products in the time between available satellite images. It could also be combined with a general spatial interpolation technique such as kriging, or satellite specific methods as described by Alvera-Azcarate *et al.* (2007).

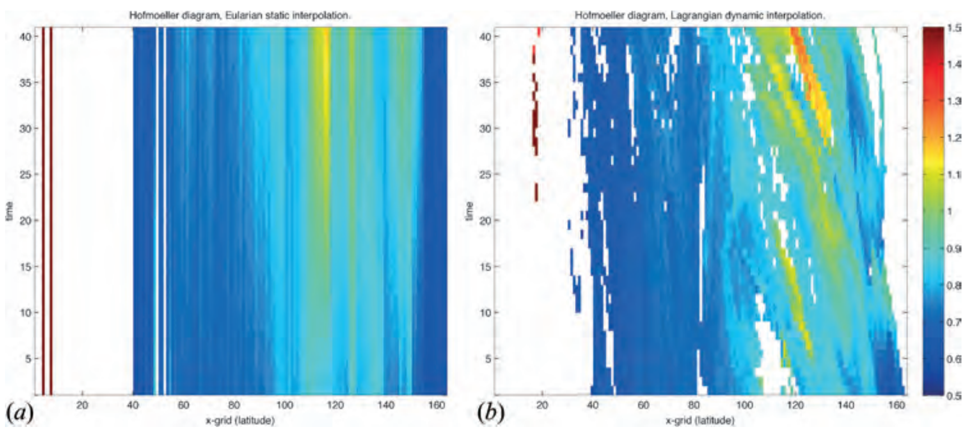

Figure 4. Hovmöller diagram showing the temporal evolution of chlorophyll along an east-west transect in the Gulf of Maine marked in 5. Satellite data is available for the region at the start and end of the time period plotted. This satellite data is interpolated in time using the two methods. For (*a*), we use the Eulerian approach to interpolate in time between the starting and ending satellite Chl_a value at every fixed location on a grid covering the Gulf of Maine. For (*b*) we use the dynamic interpolation method described: we interpolate in time along Lagrangian trajectories – between the start and end points of the modelled trajectories for which satellite data is available. Interpolation is done every three hours over a period of 5 days. In (*b*), we capture the advection of features by the circulation, which is evidenced by inclined streaks on the space-time plot, whereas (*a*) is the mere static blending of satellite fields.

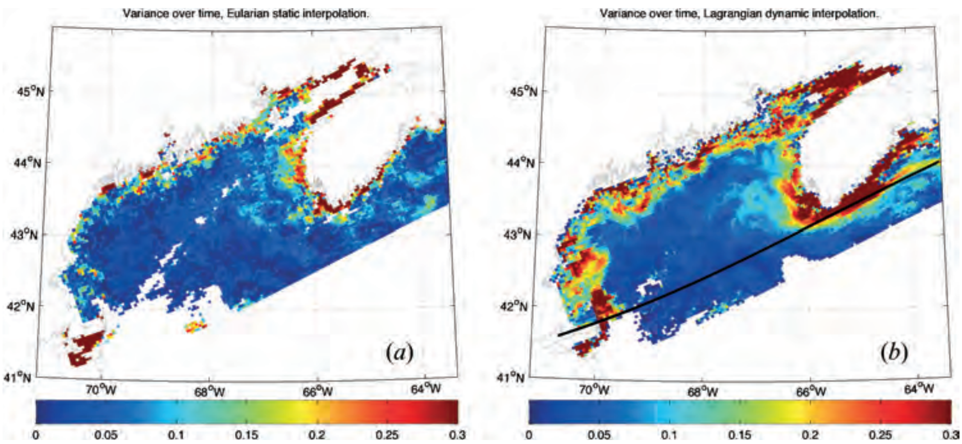

Figure 5. Variance over time in each grid cell calculated for the interpolation period between two satellite images 5 days apart. The interpolation was carried out using two methods: In (*a*) Eulerian morphing between two satellite images, and (*b*) Lagranian interpolation using particle tracing of water parcels. The temporal variability experienced at each location is considerably larger in the latter case, where the advection of features is accounted. The black line in (*b*) indicates the transect over which the Hovmöller diagrams in figure 4 are calculated.

4. Summary and discussion

The Lagrangian methodology is effective for the interpretation and interpolation of satellite data. From the biogeochemical standpoint, its greatest value is in quantifying the source/sink of properties. This method has been applied for diagnosing the net phytoplankton productivity (net community production) over a period of three years in the Gulf of Maine as described in Jönsson *et al.* (2008). This sort of synoptic, time-dependent quantification is invaluable to our understanding and assessment of the carbon cycle.

In general, the approach also enables the tracking of water masses and properties within the circulation fields. It could be used to combine data from a multitude of observing platforms into a unified framework. One could seed and advect particles representing data from buoys, AUVs, and ship measurements, providing the data sets have well defined spatial and temporal positions. It allows tracing the origin, fate, and age of water parcels, and river discharge in coastal regions. It also offers the possibility of combining land-based measurements with oceanic satellite data.

The methodology is generally applicable to any satellite fields, provided velocity fields of high fidelity are available for the region of interest. Applying the method to coastal regions would extend the value of satellite data, as well as operational coastal models and observational networks. One limitation, the vertical movement of water, will be challenging to resolve and requires further research. However in most cases, exclusive use of horizontal surface flows may be adequate for the interpretation of satellite data. Further work is needed in quantifying the error in our estimates due to imperfect trajectories. An assessment of velocity fields using satellite data would be valuable not only to our Lagrangian diagnosis, but could have wide applicability in the testing of circulation models.

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