

~~Mesoscale and Mechanisms controlling mesoscale/submesoscale physical-biological interactions: will the SWOT altimeter resolve the mechanisms controlling hotspots in net community production?~~  
export, with simulation-based studies on how to sample them

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**Short title: Hotspots in net community production and export**

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Start date: ~~January~~July 1, 2016  
Duration: ~~4~~3 years

**Outline**

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## Project Summary

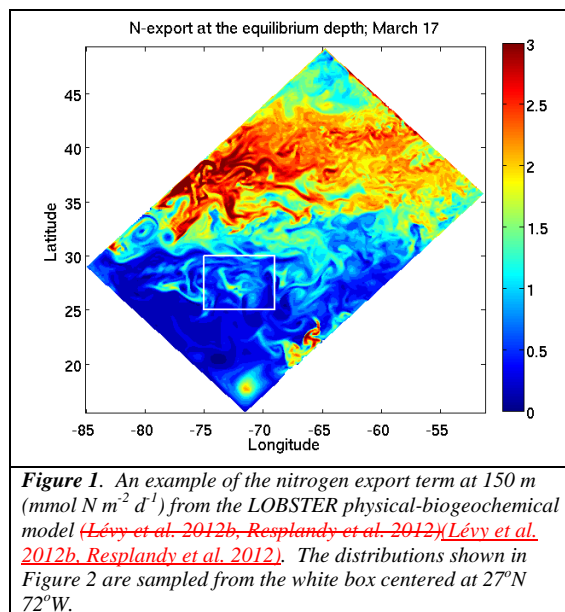
The physical, biological and geochemical processes that lead to the transfer of carbon from the surface to the deep ocean via the “biological pump” vary on a tremendously wide range of scales. Net community production (NCP) provides the fuel for the biological pump, and recent observations indicate substantial variability of NCP on spatial scales of less than 30 km (the submesoscale) and time scales of days. ~~Current altimeter missions provide the mesoscale context.~~ Large scale field experiments are currently being planned for the North Atlantic and North Pacific as part of the EXPORTS project, yet our understanding of how to grapple with these “hotspots” scales of variability in NCP, ~~but they do not resolve the essential interaction between mesoscale and submesoscale dynamics that control the underlying processes.~~ The Surface Water and Ocean Topography (SWOT) mission will provide a new window into these spatial scales that will be of enormous value to interdisciplinary studies of ocean biogeochemistry. ~~export production remains incomplete.~~ We propose to use ~~of~~ a coupled physical-biogeochemical model together with existing high-resolution measurements ~~of~~ oxygen and NCP to ~~develop a more complete understanding of~~ investigate the role of mesoscale and submesoscale processes in upper ocean ecosystem dynamics and carbon flux. This combination of observations and models will be used to assess sampling strategies for the EXPORTS field campaign, providing an objective basis on which to assess the spatial and temporal scales on which various observing assets should be deployed.

Our specific objectives are to:

1. ~~Incorporate~~ Test the oxygen dynamics ~~recently incorporated~~ into an existing biogeochemical model (LOBSTER; Lévy et al. 2012; Resplandy et al. 2012).
2. Carry out high-resolution (1/54”) coupled physical-biological simulations in an idealized North Atlantic domain.
3. Compare simulated and observed hotspots in net community production.
4. Revise the biogeochemical model as systematic discrepancies warrant.
5. Simulate sampling of environmental conditions in hotspots of net community production from the model solutions with a suite of remote sensing instruments (~~SWOT altimetry~~, ocean color, SST) using the space/time parameters specific to each platform.
6. Evaluate the accuracy with which hotspots in net community production can be reconstructed using these satellite data sets.
7. Carry out ~~observing system simulation experiments~~ Observing System Simulation Experiments (OSSEs) to provide guidance for *in situ* process studies ~~to test these ideas once the SWOT altimeter is operational~~ such as EXPORTS.

The proposed research thus incorporates multiple satellite missions together with *in situ* data and numerical models to improve our understanding of physical-biological interactions at the

mesoscale and submesoscale. ~~As such, it resonates with theme 2.2 of solicitation NNH11ZDA001N, Mesoscale and Submesoscale processes: “Both modeling and observational studies will be needed to develop ideas and methodologies to maximize the science return of SWOT observations.” Although our focus is not solely on physical oceanography and circulation per se, satellite altimetry provides the foundation for this activity. As such, we submit that the SWOT science team is an ideal environment for this interdisciplinary research. Our specific emphasis on processes regulating new production and export flux and associated sampling issues are directly relevant to theme 2.2 of solicitation NNH15ZDA001N-OBB, Global Data Sets and Modeling In Support of Planned Northeast Pacific and North Atlantic Export Flux Studies.~~



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## 1. Introduction

The “biological pump” plays a key role in regulating global climate by exporting roughly 10 Gt of carbon per year out of the euphotic zone (Falkowski et al. 1998, Volk & Hoffert 1985)(Falkowski et al. 1998, Volk & Hoffert 1985). However, measurements of export production (EP) vary by more than an order of magnitude on regional and seasonal scales, and current models poorly capture this variability (Buesseler & Boyd 2009)(Buesseler & Boyd 2009). Net community production (NCP), defined as the difference between C fixation via photosynthesis and total respiration in the euphotic zone, must balance EP over large spatiotemporal scales (basin wide, annual). However, the processes that control NCP and EP and hence their variability, are likely to occur at smaller submesoscales (SMS). ~~Current altimeter missions provide the mesoscale context for these “hotspots” in NCP, but they do not resolve the essential interaction between mesoscale and submesoscale dynamics that control the underlying processes. The Surface Water and Ocean Topography (SWOT) mission will provide a new window into these spatial scales (Fu & Ubelmann 2013) that will be of enormous value to interdisciplinary studies of ocean biogeochemistry.~~ We propose to use of a coupled physical-biogeochemical model together with existing high-resolution measurements oxygen and NCP to develop a more complete understanding of the role of mesoscale and submesoscale processes in upper ocean ecosystem dynamics and carbon flux. In addition, we plan to use our results to evaluate sampling strategies proposed for upcoming field studies of these processes as part of the EXPORTS program (Siegel et al. 2015).

## 2. Hypothesis

A key hypothesis that needs to be tested is:

**$H_0$ : Submesoscale nutrient injections stimulate phytoplankton production, increasing NCP rates, and stimulating export.**

Support for this hypothesis comes primarily from models (e.g., Lapeyre & Klein 2006, Lévy et al. 2001, Mahadevan & Archer 2000) (e.g., Lapeyre & Klein 2006, Lévy et al. 2001, Mahadevan & Archer 2000). For example, a recent submesoscale-resolving, physical-biogeochemical model suggests that the processes controlling EP and NCP respond strongly to physical forcing on timescales of days and over spatial distances on the order of tens of kilometers (Figure 1; Lévy et al. 2012a, Lévy et al. 2012b, Resplandy et al. 2012) (Figure 1; Lévy et al. 2012a, Lévy et al. 2012b, Resplandy et al. 2012). Mahadevan et al. (2012)(2012) suggest that the SMS influences the timing of the spring bloom via its role in stratification.

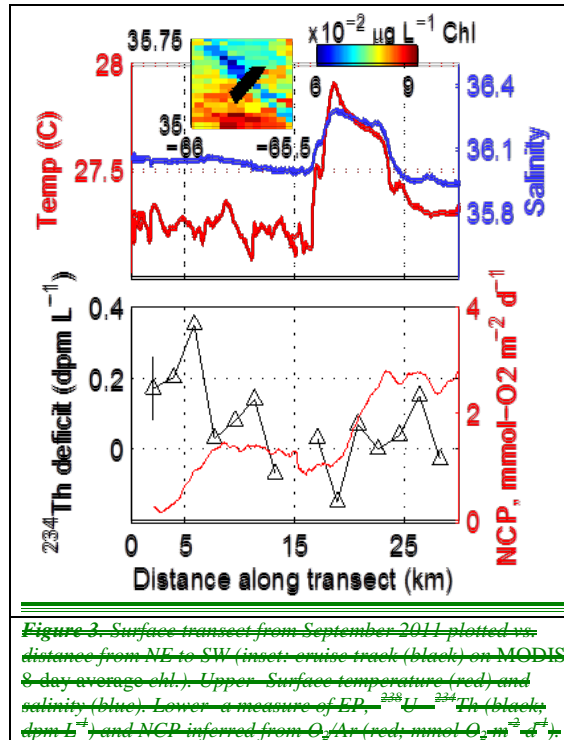


Figure 3. Surface transect from September 2011 plotted vs. distance from NE to SW (inset: cruise track (black) on MODIS 8 day average chl.). Upper: Surface temperature (red) and salinity (blue). Lower: a measure of EP,  $^{234}\text{Th}$  (black,  $\text{dpm L}^{-1}$ ) and NCP inferred from  $\text{O}_2/\text{Ar}$  (red,  $\text{mmol O}_2 \text{ m}^{-2} \text{ d}^{-1}$ ).

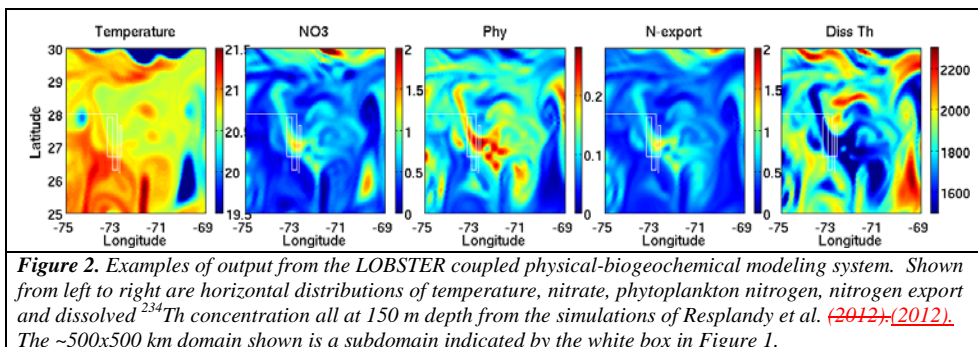


Figure 2. Examples of output from the LOBSTER coupled physical-biogeochemical modeling system. Shown from left to right are horizontal distributions of temperature, nitrate, phytoplankton nitrogen, nitrogen export and dissolved  $^{234}\text{Th}$  concentration all at 150 m depth from the simulations of Resplandy et al. (2012)(2012). The  $\sim 500 \times 500$  km domain shown is a subdomain indicated by the white box in Figure 1.

A ~~zoomed-in~~ zoom view of the simulation depicted in Figure 1 reveals intricate relationships between physical and biogeochemical variables relevant to export (Figure 2). Given the characteristic spatial scales on the order of 10 km and temporal scales of days to weeks, the practical difficulties in capturing such processes observationally are self-evident. Nevertheless, ~~some~~ important inroads have been made in that regard.

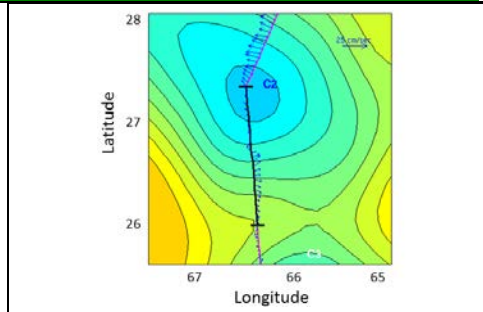
### 3. Existing observations

Observational support for the importance of submesoscale motions on ocean biogeochemistry and the ubiquitous presence of SMS features in the global ocean has come from the analysis of the divergence rate of adjacent surface water parcels (i.e., Finite Space Lyapunov Exponents [FSLE's]) using satellite altimetry (e.g., d'Ovidio et al. 2010, Waugh & Abraham 2008)(e.g., d'Ovidio et al. 2010, Waugh & Abraham 2008). Locations of SMS features observed in this manner correspond well with satellite chlorophyll distributions (Calil & Richards 2010, d'Ovidio et al. 2010, Lehahn et al. 2007)(Calil & Richards 2010, d'Ovidio et al. 2010, Lehahn et al. 2007) and even the foraging locations of frigate birds (Tew Kai et al. 2009)(Tew Kai et al. 2009) and the transport of fish larvae (Harrison et al. 2013).

Field data for EP on submesoscales ( $\leq 30$  km) show a large degree of unexplained variability in the NW Pacific (Buesseler et al. 2009, Guidi et al. 2007)(Buesseler et al. 2009, Guidi et al. 2007), NE Atlantic (Guidi et al., 2007), Southern Ocean (Rutgers van der Loeff et al. 2011)(Rutgers van der Loeff et al. 2011) and West Antarctic Peninsula (Owens 2013)(Owens 2013). In parallel, considerable SMS variability in NCP is also evident in the Southern Ocean (Hamme et al. 2012)(Hamme et al. 2012), in the subtropical Atlantic (Stanley et al. submitted)(Stanley et al. submitted), and in the surface waters of the Equatorial Pacific, with NCP tripling over a distance of just 5 km (Stanley et al. 2010)(Stanley et al. 2010).

We recently collected a one-dimensional "snapshot" of variability in both EP and NCP on 1-3 km scales in surface properties along a 30-km transect intersecting a narrow ( $< 10$  km wide), low-productivity feature located  $\sim 350$  km north of Bermuda (Figure 3). Continuous temperature and salinity data, plotted with respect to distance along the transect from NW to SE, show the cross-section of this feature, which is also visible in satellite imagery as a low-chlorophyll band perpendicular to the sampling line. Tracers for EP and NCP are spatially decoupled and exhibit significant, along-transect variability. In general, NCP is net-autotrophic and increases along with MODIS-derived chlorophyll concentrations toward the SW. Mid-transect, local minima in both NCP and chlorophyll coincide with strong physical

**Figure 3.** Surface transect from September 2011 plotted vs. distance from NE to SW (inset: cruise track (black) on MODIS 8-day average chl.). Upper- Surface temperature (red) and salinity (blue). Lower- a measure of EP,  $^{238}\text{U} - ^{234}\text{Th}$  (black;  $\text{dpm L}^{-1}$ ) and NCP inferred from  $\text{O}_2/\text{Ar}$  (red;  $\text{mmol O}_2 \text{ m}^{-2} \text{ d}^{-1}$ ).



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gradients. EP temperature and salinity data, plotted with respect to distance along the transect from NW to SE, show the cross section of this feature, which is also visible in satellite imagery as a low-chlorophyll band perpendicular to the sampling line. Tracers for EP and NCP are spatially decoupled and exhibit significant along-transect variability. In general, NCP is not autotrophic and increases along with MODIS-derived chlorophyll concentrations toward the SW. Mid-transect, local minima in both NCP and chlorophyll coincide with strong physical gradients. Export production, on the other hand, is highest towards the beginning of the transect and decreases as NCP increases. Maxima in NCP and EP are separated by a distance of ~18 km in the vicinity of strong submesoscale physical gradients, suggesting these processes are not at steady-state.

**We propose to investigate submesoscale hotspots of biogeochemical activity, and use their spatiotemporal variations to illuminate the underlying processes that control NCP (and ultimately EP).**

In the past, submesoscale features have been difficult to locate in the field, but with the addition of an O<sub>2</sub> sensor to the tow-yo'ed Video Plankton Recorder / CTD / sensor system (referred to as the VPR), we now have high-resolution cross-sections of such features (Figure 4). During a recent voyage from Bermuda to Barbados, we saw biological hotspots regularly along our cruise track (Figure 5). These are exemplified by high chlorophyll fluorescence anomalies coinciding with low O<sub>2</sub> anomalies (red circles in Figure 4b,c). Low O<sub>2</sub> (rather than high O<sub>2</sub>) is associated with these “young” hotspots likely because upwelled water carries high nutrients and an oxygen debt. Surface measurements of O<sub>2</sub>/Ar (Figure 4a) show peaks above these hotspots, illustrating that the SMS features seen at depth are often reflected in the surface record as increases in NCP. Additionally, there are peaks in the surface O<sub>2</sub>/Ar that do not appear in the VPR data, which may be remnants of “old” SMS events. These observations illustrate the importance of the temporal and vertical dimensions when sampling biogeochemical hotspots.

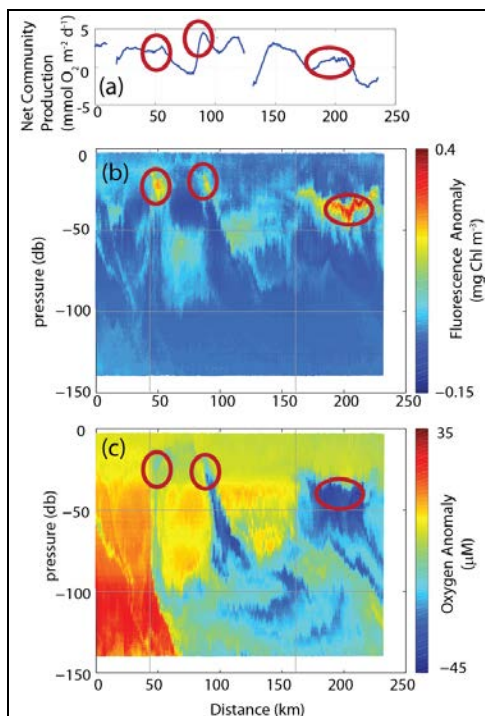
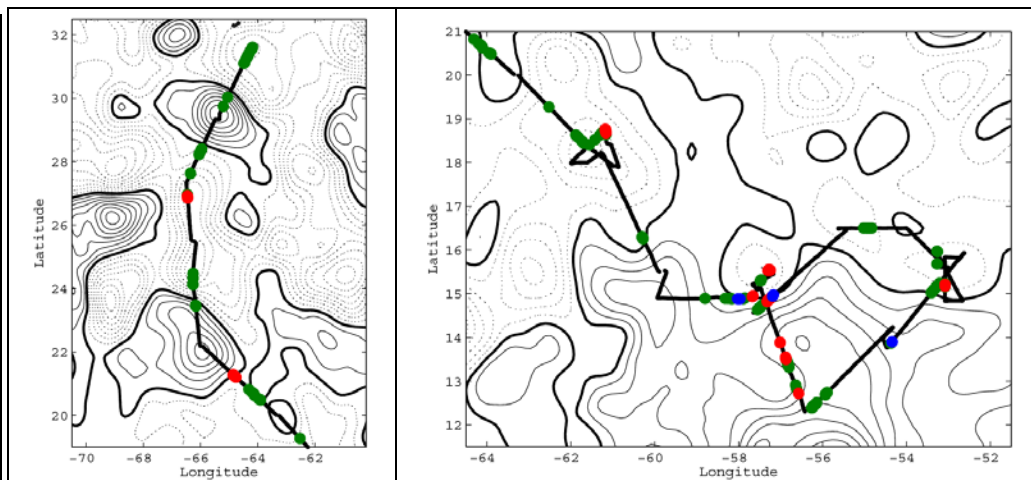
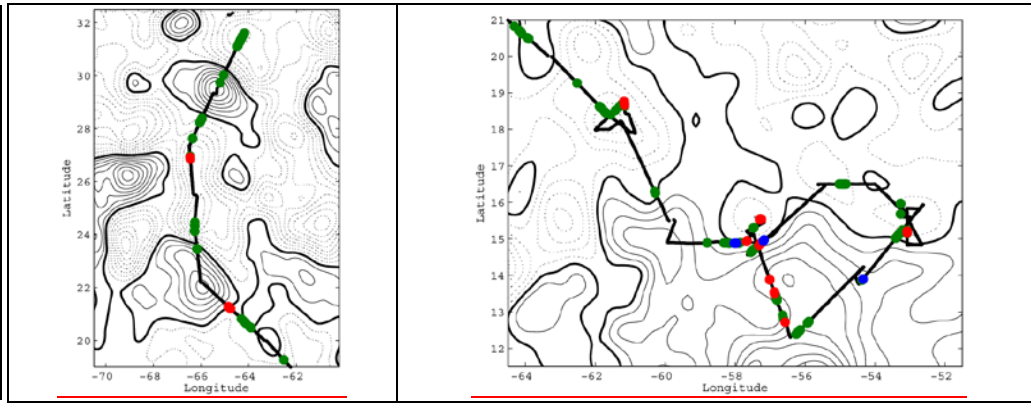


Figure 4. Top: Cruise track overlaid on satellite-based sea level anomaly. Cyclone C2 is a depression in sea level of ca. 20 cm. Blue vectors represent underway ADCP velocity measurements. Panels (a-c) below come from the black portion of the track, with endpoints indicated by hash marks. (a) NCP, as determined by O<sub>2</sub>/Ar data, in surface water measured underway during a 250 km transect. (b) and (c): fluorescence and O<sub>2</sub> anomalies measured by the VPR on the same transect. Biological hotspots circled in red are shown in all three records.

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*Figure 5. VPR tows from R/V Oceanus voyage 471 (April/May 2011) overlaid on satellite derived sea level anomaly (positive contours solid, negative contours dashed, zero contour bold; contour interval 2.5 cm). The cruise track is split into two segments to facilitate higher resolution. Locations of biological hotspots identified in the data are indicated by dots, with red dots indicating major hotspots where change in oxygen is negative compared to water of the same temperature and salinity, and blue dots indicating major hotspots where the change in oxygen is positive compared to water of the same temperature and salinity. Green dots represent minor hotspots, i.e. those with smaller anomalies in O<sub>2</sub> and fluorescence. From Stanley and McGillicuddy (submitted).*

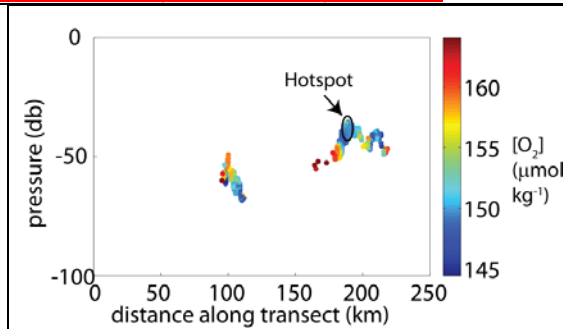
It is worth noting the low O<sub>2</sub> characteristic of the hotspots we observed may be due at least in part to increased respiration, perhaps even negative NCP. In order to quantify the change in oxygen in a hotspot, one needs to know the initial oxygen concentration prior to upwelling. Unfortunately, in the recent voyage, we only had information from single transects through three-dimensional fields that were evolving

**Figure 5.** VPR tows from R/V Oceanus voyage 471 (April/May 2011) overlaid on satellite-derived sea level anomaly (positive contours solid, negative contours dashed, zero contour bold; contour interval 2.5 cm). The cruise track is split into two segments to facilitate higher resolution. Locations of biological hotspots identified in the data are indicated by dots, with red dots indicating major hotspots where change in oxygen is negative compared to water of the same temperature and salinity, and blue dots indicating major hotspots where the change in oxygen is positive compared to water of the same temperature and salinity. Green dots represent minor hotspots, i.e. those with smaller anomalies in O<sub>2</sub> and fluorescence. From Stanley and McGillicuddy (submitted).

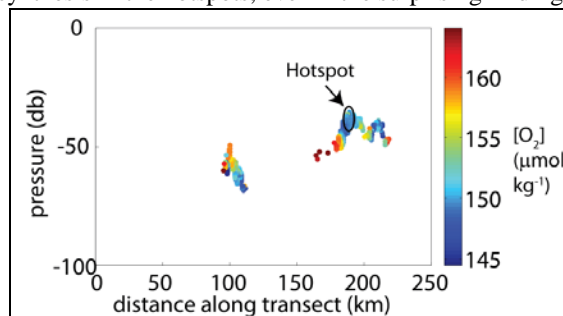
in time. Therefore, we cannot unequivocally determine the source waters for each hotspot. However, we can make a crude attempt to do so by calculating the oxygen concentration of water with the same density, temperature, and salinity as that of the hotspot (Figure 6). When we do so, we find very surprisingly that in two-thirds of the hotspots we analyzed, oxygen appears to be decreasing (red circles in Figure 5)

compared to the likely source water. Only in one-third of the hotspots analyzed was H<sub>0</sub> borne out (blue circles in Figure 5). Thus – if this crude analysis is correct – there is often actually negative NCP in the hotspots, contrary to our hypothesis H<sub>0</sub>. Such negative NCP could occur if photosynthesis were indeed stimulated in the hotspots due to upwelled nutrients, as we hypothesize in H<sub>0</sub>, but if respiration was stimulated to a greater extent. To test this, we will ultimately need to measure NCP in hotspots that we follow in space and time, making definitive observations of the source of the upwelled water. Additionally, measurements of gross primary production (which is equal to only the photosynthetic flux) made in the hotspots will allow us to determine if there really is increased photosynthesis in the hotspots, even if the surprising finding of negative NCP is confirmed. Clearly

there is great need to further examine hotspots to determine the sign and the magnitude of the change in NCP and gross primary production due to these ubiquitous features. ~~The SWOT altimeter will provide unprecedented context for coupled physical biological studies of this type, and the proposed modeling study will lay the necessary groundwork by (1) making extensive use of available data and models to understand the dynamics, and (2) planning definitive field experiments to test the ideas, and to elucidate their impacts on export.~~



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**Figure 6.** Oxygen concentration along a constant temperature and salinity surface ( $T=26.32\text{ }^{\circ}\text{C}$ ,  $S=35.77\text{ psu}$ ) matching that of the hotspot located at approximately 200 km (circled in black) on the VPR tow shown in Figure 4. Note that the oxygen concentration within the hotspot is on average lower than other oxygen concentrations of the same temperature and salinity. Thus the calculated change in oxygen is negative for this hotspot, therefore surprisingly suggesting negative NC. However, uncertainties remain on whether water with the same temperature and salinity is truly the source water for the hotspot. From Stanley and McGillicuddy (submitted).



#### 4. Proposed research

We propose to use of a coupled physical-biogeochemical model together with existing high-resolution measurements oxygen and NCP to develop a more complete understanding of the role of mesoscale and submesoscale processes in upper ocean ecosystem dynamics and carbon flux. Our seven specific objectives ~~are to follow below; each is described in detail in subsequent sections.~~

*Figure 6. Oxygen concentration ( $\mu\text{mol kg}^{-1}$ ) along a constant temperature and salinity surface ( $T=26.32^\circ\text{C}$ ,  $S=35.77$  psu) chosen to match that of the hotspot located at approximately 200 km (circled in black) on the VPR tow shown in Figure 4. Note that the oxygen concentration within the hotspot is on average lower than other oxygen concentrations of the same temperature and salinity. Thus the calculated change in oxygen is negative for this hotspot, therefore surprisingly suggesting negative NCP and hence excess of respiration over photosynthesis. However, uncertainties remain on whether water with the same temperature and salinity is truly the source water for the hotspot. From Stanley and McGillicuddy (submitted).*

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1. ~~Incorporate~~Test the oxygen dynamics recently incorporated into an existing biogeochemical model (LOBSTER; Lévy et al. 2012; Resplandy et al. 2012).
2. Carry out high-resolution ( $1/54^\circ$ ) coupled physical-biological simulations in an idealized North Atlantic domain.
3. Compare simulated and observed hotspots in net community production.
4. Revise the biogeochemical model as systematic discrepancies warrant.
5. Simulate sampling of environmental conditions in hotspots of net community production from the model solutions with a suite of remote sensing instruments (SWOT altimetry, ocean color, SST) using the space/time parameters specific to each platform.
6. Evaluate the accuracy with which hotspots in net community production can be reconstructed using these satellite data sets.
7. Carry out observing system simulation experiments (OSSEs) to provide guidance for *in situ* process studies ~~to test these ideas once the SWOT altimeter is operational~~such as EXPORTS.

~~Each of these is described in turn below.~~

##### 4.1 ~~Incorporate~~Test the oxygen dynamics recently incorporated into an existing biogeochemical model

The proposed research will be based on the LOBSTER model (~~Lévy et al. 2012b, Lévy et al. 2010, Resplandy et al. 2012~~)(Lévy et al. 2012b, Lévy et al. 2010, Resplandy et al. 2012). LOBSTER is an ecosystem/biogeochemistry model based upon a phytoplankton-zooplankton-detritus-ammonium-nitrate-labile DOM nitrogen cycle model with modules for  $\text{CO}_2$  air-sea fluxes and  $^{234}\text{Th}$  scavenging and export (~~Karleskind et al. 2011, Lévy et al. 2012b, Resplandy et al. 2009, Resplandy et al. 2012~~)(Karleskind et al. 2011, Lévy et al. 2012b, Resplandy et al. 2009, Resplandy et al. 2012). ~~Our first task will be to add oxygen dynamics to the model (LOBSTER-oxy), which will be straightforward because the biogeochemical and gas exchange modules are already in place—they will simply need to be adapted to include this additional variable using~~

~~Redfield stoichiometry.~~ Oxygen dynamics were recently added to the model (LOBSTER-oxy), utilizing the biogeochemical and gas exchange modules that were already in place. Redfield stoichiometry is implicit in this formulation. Although we are confident that the new coding is robust, it is incumbent upon us to verify that the model is capable of accurately simulating the regime of interest. For the present purposes, the Bermuda Atlantic Time-series Site (BATS) is an ideal testbed, as the seasonal cycle of oxygen is well documented from both observational and modeling perspectives (Jenkins & Goldman 1985, Musgrave et al. 1988, Nicholson et al. 2012, Ono et al. 2001, Spitzer & Jenkins 1989).

#### 4.2. Carry out high-resolution (1/54°) coupled physical-biological simulations in an idealized North Atlantic domain.

We will run ~~a bio-coupled~~ physical ~~simulation biological simulations~~ in an idealized North Atlantic domain. The physical model is the primitive equation ocean circulation model NEMO (Nucleus for European Modeling of the Ocean) (~~Madec 2008~~)(Madec 2008). The horizontal grid resolution is 1/54°, which permits description of the mesoscale and sub-mesoscale features of the flow with an effective resolution of 1/9° (~~Lévy et al. 2012b~~)(Lévy et al. 2012b). There are 30 vertical levels. The model domain (Figure 1) is a rectangle of dimensions 2000 km x 3000 km, of 4 km depth, rotated by 45° on the beta-plane, with closed boundaries and forced at the surface with seasonal buoyancy fluxes and wind. This configuration features a seasonally varying, semi-realistic Northwest Atlantic with a baroclinically unstable jet (the model's Gulf Stream) separating a warm, oligotrophic subtropical gyre south of the jet from a colder and more productive subpolar gyre north of it (see Lévy et al. 2010 and Lévy et al. 2012 for full details on the model). Instability processes lead to mesoscale turbulence characterized by a large number of interacting mesoscale eddies and submesoscale fronts. This physical model configuration was previously used alone or in association with different ecosystem models to examine various aspects of the impact of mesoscale turbulence, such as the large-scale ocean circulation (~~Lévy et al. 2010~~)(Lévy et al. 2010), large-scale nutrient budgets (~~Lévy et al. 2012b~~)(Lévy et al. 2012b), organic export (~~Resplandy et al. 2012~~)(Resplandy et al. 2012), biogeochemical eddy-reactions (~~Lévy & Martin 2013~~)(Lévy & Martin 2013), internal variability (~~Lévy et al. 2014b~~)(Lévy et al. 2014b), Redfield ratios (~~Ayata et al. 2014~~)(Ayata et al. 2014) and phytoplankton diversity (~~Lévy et al. 2014a~~)(Lévy et al. 2014a). Here, we will run this physical model with LOBSTER-oxy online. The reason for choosing this model configuration is because its reduced dimension (rather than a full North Atlantic domain) will allow us to undertake ~~a long simulations~~ simulations at high resolution, which will be necessary to equilibrate the oxygen concentration of subsurface waters. The model will resolve the seasonal cycle and variability in biology over spatial scales ranging from 1000 km down to 10 km.

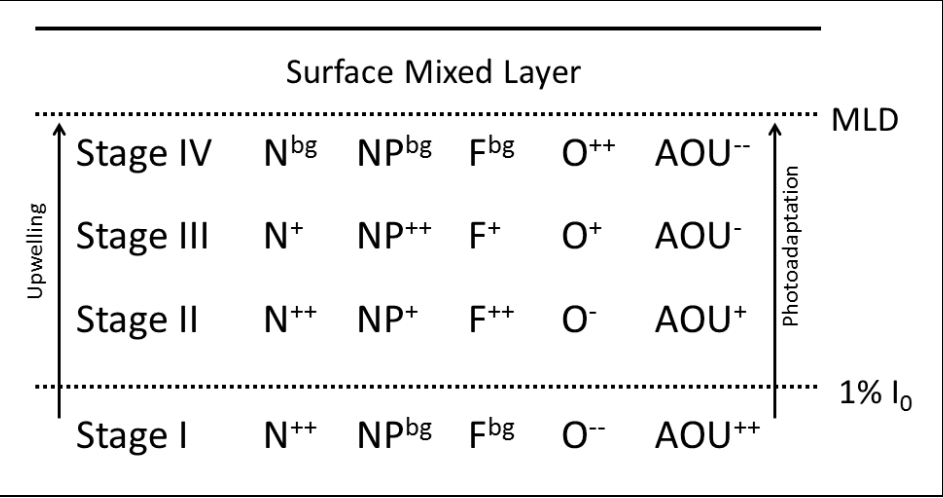
#### 4.3. Compare simulated and observed hotspots in net community production.

It is important to note that the LOBSTER model is a process model and is *not* meant to depict the specific conditions we observed (Figures 3-6); rather its use enables us to concentrate on phenomenological aspects of our problem and to apply it as a synthesis tool. Specifically, we will use the LOBSTER model to compare the phenomenology we observed with model output. In the latter activity, we will identify submesoscale hotspots in the model that resemble our observations, and use the model to carry out detailed term-by-term analysis of the underlying dynamics—an approach that is made possible by the space-time continuous fields from the model solution. This analysis will be conducted in both in ~~eulerian~~ Eulerian coordinates ~~as well~~

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**Figure 7. Conceptual model of the nutrient (N), new production (NP), fluorescence (F), oxygen (O), and apparent oxygen utilization (AOU) anomalies resulting from a submesoscale upwelling event.** Superscript “bg” indicates background conditions, whereas “+” and “-” signs indicate increasingly positive and negative anomalies, respectively. Depths of the mixed layer (MLD) and euphotic zone (1%  $I_0$ ) are depicted as dotted lines; the ocean surface is the bold line.

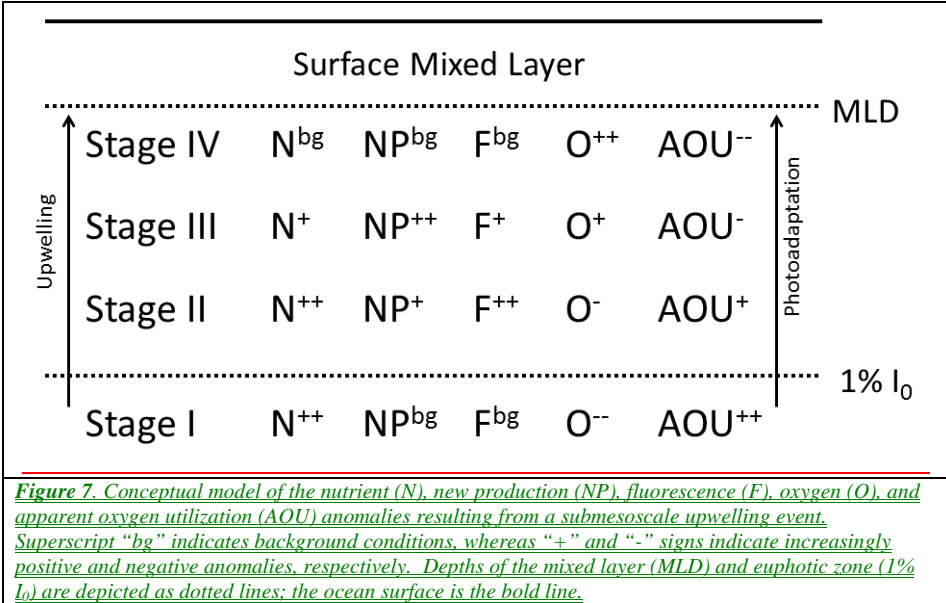
as in ~~lagrangian~~and Lagrangian frameworks following the transport pathways of ~~parcels of~~ upwelled fluid parcels that create the hotspots.



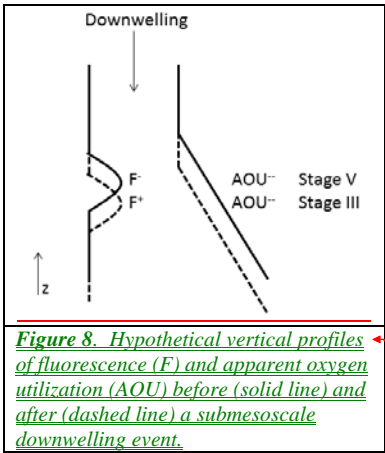
Underlying our analysis is a conceptual model of the nutrient (N), new production (NP), fluorescence (F), oxygen (O), and apparent oxygen utilization (AOU) anomalies that result from a submesoscale upwelling event (Figure 7; note that a negative AOU anomaly is associated with an increase in NCP). Stage I reflects the pre-upwelling conditions below the euphotic zone, in which nutrients are in abundance, oxygen is low, and light is insufficient for NCP (NP and F both at background). As the water parcel upwells (Stage II), nutrients are introduced into the euphotic zone which stimulates new production, increasing both fluorescence and oxygen—but there are subtleties in the two latter aspects: (1) the fluorescence anomaly is enhanced by the high chlorophyll:carbon ratio characteristic of phytoplankton inhabiting the low-light conditions of the base of the euphotic zone; and (2) although the oxygen content of the water parcel increases as a result of new production, it is still low in oxygen relative to surrounding waters; in a sense, the oxygen anomaly has become less negative. As the parcel continues to upwell (Stage III), higher light conditions stimulate more new production, removing nutrients and increasing oxygen. The higher light environment accommodates lower chlorophyll:carbon ratios, thereby lessening the fluorescence anomaly. As the upwelled nutrients become exhausted (Stage IV), new production and fluorescence return to background levels, with the positive oxygen anomaly providing the only detectable biogeochemical signature of the submesoscale upwelling event.

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In this portrayal of the conceptual model, the imprint of the upwelling does not outcrop into the mixed layer. This is of course an oversimplification, because we know that they most certainly do (Figure 4). The primary reason for initially targeting the subtropics in the summer is to examine an environment where the surface mixed layer and euphotic zone are sufficiently decoupled to allow this cascade of processes to unfold in the stratified area beneath the mixed layer, where they will be less subject to strong time-dependence in entrainment and detrainment.



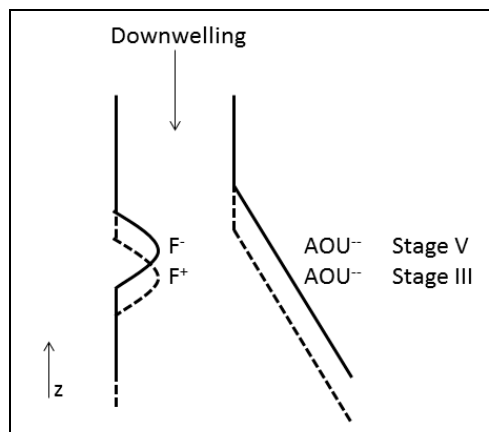
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Another complication arises in the interpretation of the conceptual model in the downwelling case (Figure 8). In the presence of a subsurface fluorescence maximum, downwelling produces vertically-adjacent anomalies of opposite sign. When coupled with the associated anomalies in AOU, this introduces a new category of perturbation which we refer to as Stage V: a negative fluorescence anomaly together with a negative AOU anomaly. Further complicating matters, the depth interval just below consists of a positive fluorescence anomaly in combination with a negative AOU anomaly, which is indistinguishable from Stage III in the upwelling case (cf. Figures 7,8).

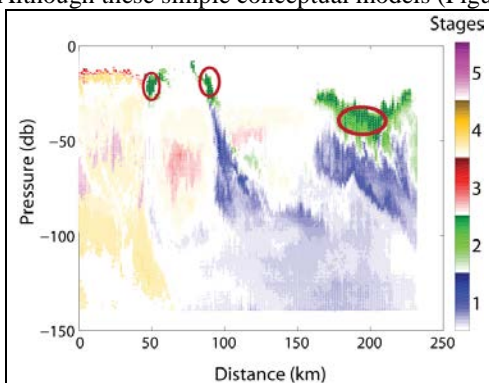


#### 4.4. Revise the biogeochemical model as systematic discrepancies warrant

We can use the magnitudes and signs of the AOU and fluorescence anomalies to diagnose the spatial distribution of our conceptual model stages relative to the observed hotspots. Figure 9 provides an example based on the preliminary data presented in Figure 4. Analyzing the complete data set in aggregate (Figure 5), we find that most of the observed hotspots are in stage 2. We sometimes see the progression from stage 1 to stage 2 but have not observed the progression from stage 2 to stage 3. Is this because we have not followed a hotspot for long enough? Or is it because respiration actually increases more than photosynthesis, perhaps due to bacteria responding more strongly to nutrient injection or to zooplankton favoring hotspots as feeding locations? Or maybe this reflects the intrinsic four-dimensionality of the process, and the particular stage 3 water parcels we encountered were not spatially connected in the along-track direction of the two-dimensional transects we collected?

Once again, this highlights the need for truly four-dimensional surveys of submesoscale features. Although these simple conceptual models (Figures 7,8) are depicted in one dimension, they are

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**Figure 9.** Stages of the conceptual model (as defined in Figures 12 and 13) as diagnosed from the magnitudes and signs of AOU and fluorescence anomalies measured in the transect shown in Figure 4. Locations of the hotspots are circled in red.

played out in a fully three-dimensional field that is evolving in As such, the alongtrack sections of we have gathered (Figure 4) do not sufficient information to test these conceptual models. The LOBSTER biogeochemical model provides an framework in which to evaluate the conceptual model more fully. If it out that the numerous hotspots of NCP we observed cannot be explained by three-dimensional

**Figure 8.** Hypothetical vertical profiles of fluorescence (F) and apparent oxygen utilization (AOU) before (solid line) and after (dashed line) a submesoscale downwelling event.

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transects, we will incorporate additional dynamics into the model. Candidate processes include zooplankton aggregation or enhanced bacterial activity, both of which could potentially increase respiration over photosynthesis, at least on a temporary basis.

#### 4.5. Simulate sampling of environmental conditions in hotspots of net community production from the model solutions with a suite of remote sensing instruments (SWOT altimetry, ocean color, SST) using the space/time parameters specific to each platform.

Our model solutions will provide realistic representations of submesoscale hotspots in net community production, highly resolved in both space and time. From these solutions, we will identify a set of approximately ten representative examples of the features of interest. We will then assess the degree to which such features can be observed via remote sensing by sampling the model solutions with measurement parameters characteristic of the various platforms. ~~The SWOT Simulator for Ocean Science<sup>†</sup> provides an ideal tool for making this assessment for SSH. As stated in the documentation, this software ingests model-produced SSH to generate “SWOT-like outputs on a swath along the orbit ground track and adds measurement error and noise, which are generated according to technical characteristics published by the SWOT project team. Not designed to directly simulate the payload instrument performance, this SWOT simulator aims at providing statistically realistic outputs for the science community with a simple software package released as an open source in Python.” For example, we will extract simulated sea level anomaly along the ground tracks of ongoing altimeter missions, map the simulated data, and compare with the original model solution. Although two-dimensional maps of sea level anomaly derived from current altimeter missions do not resolve submesoscale features, there is some submesoscale information in the alongtrack data that could prove useful. Moreover, it will be valuable to better understand the relationship between submesoscale hotspots and the larger mesoscale context. Analysis of Finite Size Lyapunov Exponents (Buesseler 2012, d'Ovidio et al. 2009, Nencioli et al. 2013, Waugh & Abraham 2008) has been particularly valuable in that regard, and thus we intend to compute them both in our model solutions and simulated data.~~

We will tailor similar measurement simulators for other platforms including ocean color and SST (Figure 10). Of course a key issue with those data streams is obscuring of the field of view by clouds, and we will use characteristic cloud masks from prior imagery of the region to provide realistic assessments of the spatial coverage and temporal resolution that can be expected. Of particular interest will be the degree to which the hydrodynamic and biological processes associated with these hotspots are manifested in surface (SST) and near-surface (ocean color) properties. The latter aspect is a bit more subtle than the prior, given that the chlorophyll signal observed by satellite generally reflects an integral over the top 1-2 optical depths (~~Gordon & McCluney 1975~~Gordon & McCluney 1975, Smith 1981).

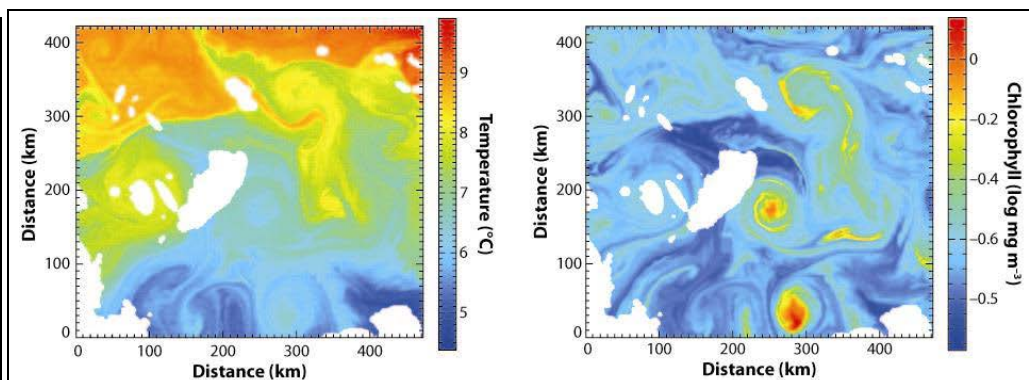
~~Incidentally, it is interesting to consider the prospect of conducting the EXPORTS field work in the North Atlantic in the context of observations from the Surface Water and Ocean Topography (SWOT) mission (Fu et al. 2012, Fu & Uebelmann 2013) planned for launch in 2020. Resolution of the SWOT altimetric measurements will be sufficient to sample the submesoscale, thereby providing a new window into these spatial scales that will be of enormous value to interdisciplinary studies of ocean biogeochemistry. If the timelines for SWOT and EXPORTS~~

<sup>†</sup> <http://sourceforge.net/projects/swotsimulatorforoceanscience>

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**Figure 10.** Sea surface temperature (left) and ocean color images (right) from satellite data (From Klein and Lapeyre (2009)(2009), images courtesy of Jordi Isern-Fontanet). Both images reveal a continuum of scales from the mesoscale to submesoscale; in particular note the submesoscale hotspots in chlorophyll that appear at fronts and around the peripheries of eddies.

appear to be compatible during the time period in which we are conducting this analysis, we will most certainly include the SWOT simulator<sup>2</sup> in our experiments.

#### 4.6. Evaluate the accuracy with which hotspots in net community production can be reconstructed using these satellite data sets.

Comparison of the simulated remote sensing measurements described in section 4.5 with the corresponding features in the full-resolution model output will provide a basis on which to evaluate the accuracy of inference derived from satellite observations alone. For example, based on the data we have in hand (Figures 4-6), it appears that the biological response to submesoscale upwelling can take place deep in the euphotic zone—as has been observed for mesoscale processes (Gaube et al. 2013, McGillicuddy et al. 2001, Siegel et al. 2008, Siegel et al. 2011)(Gaube et al. 2013, McGillicuddy et al. 2001a, Siegel et al. 2008, Siegel et al. 2011). On the other hand, surface expressions of hotspots in net community production have clearly been observed (Figure 4a). In any case, we expect that the relationships amongst SSH, SST, and ocean color in such features will be complex and depend significantly on ambient conditions, especially the depth of the mixed layer. In particular, we expect that when the mixed layer is deep, SST and ocean color measurements will more accurately represent conditions throughout the euphotic zone. With a suitably large set of representative examples, we will be able to estimate the accuracy with the associated net primary productivity (NPP) can be assessed from satellite-derived chlorophyll estimates (e.g., Behrenfeld & Falkowski 1997)(e.g., Behrenfeld & Falkowski 1997). Following the method of Nevison et al. (2012), we will estimate export production (EP) based on the Laws (2004) model relating EP to NPP and SST, and use EP as a proxy for net community production.

#### 4.7. Carry out ~~observing system simulation experiments~~ **Observing System Simulation Experiments (OSSEs)** to provide guidance for in situ process studies ~~to test these ideas once the SWOT altimeter is operational~~ **such as EXPORTS.**

<sup>2</sup> <https://sourceforge.net/projects/swotsimulatorforoceance/>

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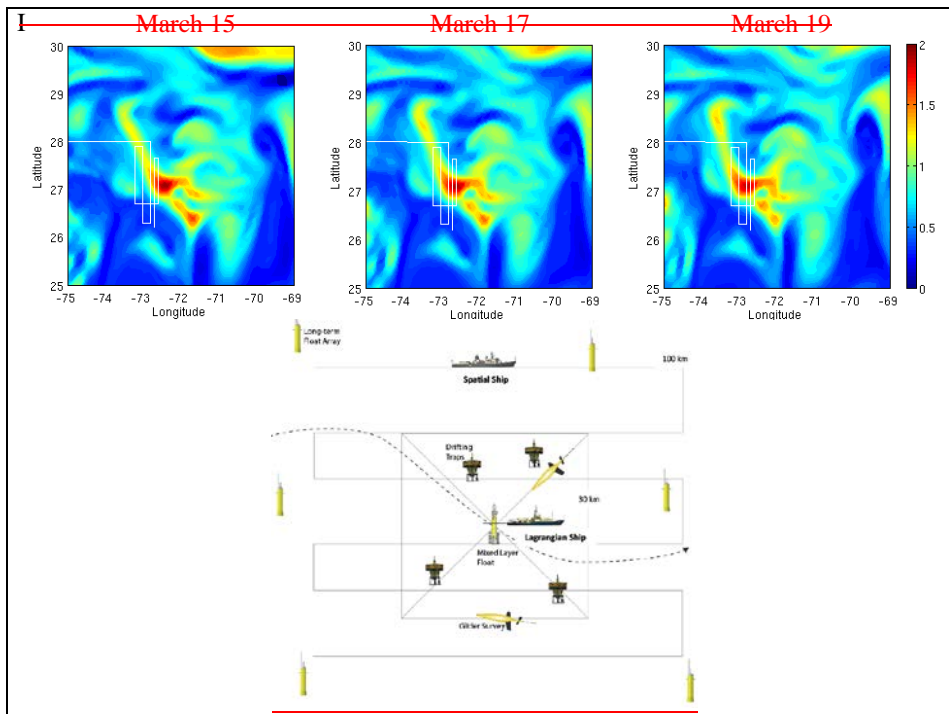
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the biological pump, observations of the four-dimensional (space-time) evolution of these features are required. High resolution altimetry from SWOT is precisely what is needed to provide real time information for siting of such studies. Expected positions of SMS fronts could be further refined by analysis of Finite Size Lyapunov Exponents (FSLEs; Buesseler 2012, d'Ovidio et al. 2009, Nencioli et al. 2013, Waugh & Abraham 2008), which we expect will be much more precise than FSLEs estimated from current altimeter products. Based on this information, towed instrument systems (such as the Video Plankton Recorder or Moving Vessel Profiler) could be used to map out hotspots and follow their temporal evolution. Surveys with towed instrumentation could be enhanced with hydrographic sampling with discrete water samples for the entire suite of variables needed to constrain NCP. This is a primary objective of the EXPORTS field program, for which a multiscale combined Eulerian / Lagrangian sampling program is envisioned (Figure 11). There will be shipboard surveys, floats, gliders, and drifting sediment traps—but the details of the sampling strategy and its effectiveness in dealing with the submesoscale remain to be worked out.



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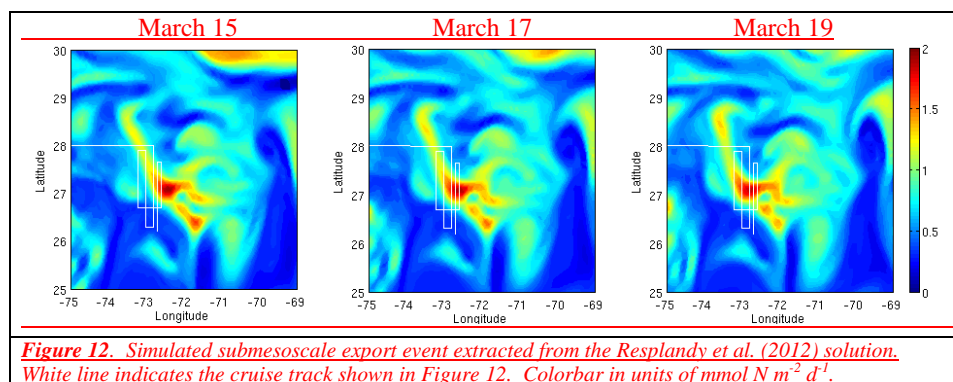
**Figure 11.** Simulated submesoscale export event extracted from the Resplandy et al. (2012) solution. White line indicates the cruise track shown in Figure 12. Colorbar at the right pertains to all three fields, in units of  $\text{mmol N m}^{-2} \text{d}^{-1}$ . **Figure 11.** Cartoon of a typical EXPORTS field deployment. A Lagrangian ship measuring rates and time-series of stocks follows a mixed layer float. A spatial ship provides spatial information on biogeochemistry as well as performing submesoscale physical oceanographic surveys. The spatial ship spatial observations are supplemented with glider surveys about the Lagrangian ship and a suite of profiling floats. The floats also provide a long-term context for the experiments. From Siegel et al. (2015).

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ulation Experiments (OSSEs) provide a powerful approach to sampling design questions of this type. This technique has its origins in dynamic meteorology (Arnold & Dey 1986, Charney et al. 1969) and is recognized as an important tool for the development of oceanographic sampling systems (Malanotte-Rizzoli 1996, McGillicuddy et al. 2001b, Robinson et al. 1998, Smith 1993). The effectiveness of any sampling strategy is ultimately determined by the accuracy with which the observations can be used to reconstruct reality—the state of the natural system being measured. In this context, reality is an elusive metric, for property distributions in the ocean rarely (if ever) have been oversampled. Given the dearth of opportunity for testing sampling strategies against objective criteria with purely observational means, OSSEs offer an attractive framework for investigation of these issues.

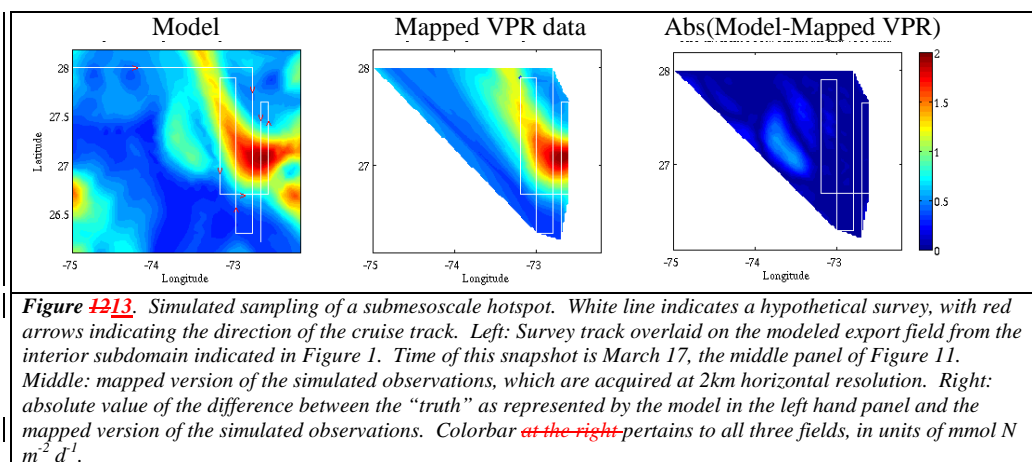
The approach begins with the construction of a simulation that is characteristic of the natural system. The model run serves as a space/time continuous representation of reality, which is then subsampled in a specified fashion to produce a simulated data set. The simulated data are then fed into an analysis scheme in which they are synthesized into a reconstruction of reality. Comparison of the reconstructed field with the “truth” as defined by the original simulation thus provides a quantitative evaluation of that particular sampling strategy and the associated analysis scheme. Of course there is an important caveat to such an evaluation: the OSSEs are based on simulations that are imperfect representations of the natural system. Thus, care must be taken to restrict the scope of the OSSEs to aspects of the model that are realistic.

To illustrate a hypothetical sampling strategy, for towed instrument systems (such as the Video Plankton Recorder or Moving Vessel Profiler), we zoom in on a subdomain of the basin scale LOBSTER model (Resplandy et al. 2012) (Resplandy et al. 2012) containing an active SMS event which is representative of the types of features we are interested in (Figure 14.12). Three snapshots at 2-day temporal resolution illustrate the westward propagation and temporal evolution of the feature. Although the spatial structure of the feature is assumed to be unknown in this sampling exercise, we assume its characteristics will be discernible with ~~our~~ the towed systems’ chlorophyll fluorescence, beam attenuation, and dissolved oxygen sensors. This facilitates construction of an **Observing System Simulation Experiment (OSSE)**, in which we extract simulated observations from the model solution in both space and time (Figure 14.13, left). Entering the sampling domain eastbound at 28°N, we encounter the frontal feature oriented NNE-SSW. Upon crossing the feature and seeing conditions return to the background state, we turn 90° to the right, putting us on a southward course. In this transect we pass through the region of highest export, but we do not encounter the absolute peak. We turn 90° to the right, steam 20 km to the west, and then turn 90° to the right again for a northward transect. Again we encounter the heart of the feature, but its magnitude is slightly less than we observed to the east. As soon as we hit background conditions again, we delimit the feature to the west by making a turn to the left, steaming 20 km to the west, and then returning on a southbound transect. Once in background conditions again, we turn eastward and continue until we are 20 km east of the easternmost line and occupy a northbound transect until we hit background conditions again.



Because the peak we observe on this transect is lower than the previous peak, we turn westward and then southward to occupy a line half way in between the two lines. This results in a near-direct hit on the peak of the feature, which then becomes the reference point for subsequent process studies. The total cruise track is 1084 km, requiring 58 hours to complete at a speed of 10 knots.

We analyze the efficacy of our sampling strategy by mapping the simulated observations (Figure 4213, middle) and comparing them with the “truth” as defined by the model output at the central time (Figure 4213, left) to quantify the difference between the two (Figure 4213, right). From these results it is clear that the survey identifies and delineates the edges of the feature by systematically changing direction whenever local, biogeochemical maxima (as measured by



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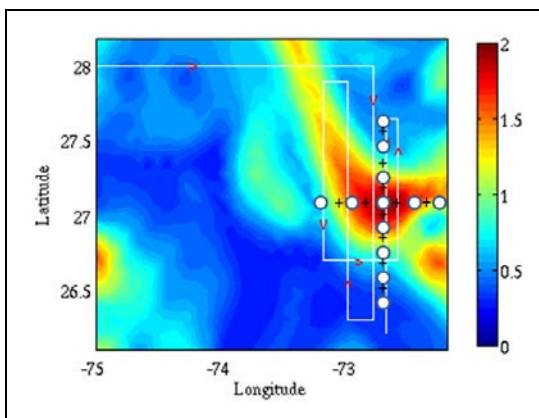
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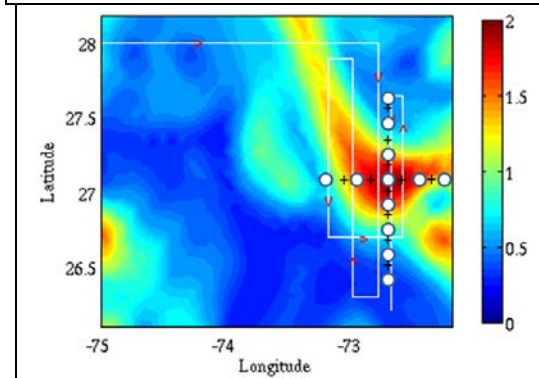
underway and towed sensors) are encountered adjacent to background-level signals. Although the underlying field evolves in space and time during the survey, this strategy is sufficient to provide a synoptic realization of the SMS hotspot. Significant differences between the mapped observations and the “truth” are mostly confined to an area west of the survey tracks, which simply reflects the uncertainty in extrapolation of the mapped field outside the domain of the observations—portions of the map which of course would not be utilized in post-cruise analysis. Of course we recognize that the conclusions from this OSSE are only as valid as the model simulation on which it is based. Even though the resolution of the underlying model is among the finest published to date for such regimes, it does not contain the full range of scales present in the real ocean. Nevertheless, the OSSE gives us confidence we can gather quasi-synoptic snapshots of SMS hotspots, at least insofar as they are represented in a state-of-the-art model.

This initial OSSE provides a very simple example, which we propose to expand using more variables and a variety of sampling techniques (e.g. Figure 13, 14). For example, NCP can be determined *in situ* from geochemical tracers such as  $O_2/Ar$  (e.g., Craig & Hayward 1987, Emerson et al. 1991, Spitzer & Jenkins 1989) (e.g., Craig & Hayward 1987, Emerson et al. 1991, Spitzer & Jenkins 1989) and DIC drawdown (e.g., Bates et al. 2005, Gruber et al. 1998, Mathis et al. 2009, Mathis et al. 2010, Quay & Stutsman 2003) (e.g., Bates et al. 2005, Gruber et al. 1998, Mathis et al. 2009, Mathis et al. 2010, Quay & Stutsman 2003).

In this work, we will evaluate our ability to estimate NCP in the hotspots by measuring the  $O_2/Ar$  of discrete bottle samples ( $n \sim 500$ ) filled with water collected on the CTD casts targeting the hotspots. We also will examine the efficacy of a shipboard equilibrator mass spectrometer fed by the underway seawater system in order to continuously quantify NCP in the mixed layer with several km resolution. In our prior observations, the deep hotspots have been expressed in the



**Figure 13.** Simulated sampling of a submesoscale export event. White line indicates a hypothetical towed survey, with red arrows indicating the direction of the cruise track, as shown in the left panel of Figure 8. Hydrographic stations occupied after the completion of the towed survey are shown as black plus signs (CTD only) and white dots (water samples taken). Colorbar at the right is in units of  $mmol\ N\ m^{-2}\ d^{-1}$ .



**Figure 14.** Simulated sampling of a submesoscale export event. White line indicates a hypothetical towed survey, with red arrows indicating the direction of the cruise track, as shown in the left panel of Figure 8. Hydrographic stations occupied after the completion of the towed survey are shown as black plus signs (CTD only) and white dots (water samples taken). Colorbar at the right is in units of  $mmol\ N\ m^{-2}\ d^{-1}$ .

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mixed layer as peaks in NCP (Figure 4a).

The O<sub>2</sub>/Ar approach takes advantage of the similar solubility (~~Garcia & Gordon 1992, Hamme & Emerson 2004, Weiss 1970~~)(Garcia & Gordon 1992, Hamme & Emerson 2004, Weiss 1970) and molecular diffusivity (~~Jähne et al. 1987~~)(Jähne et al. 1987) of O<sub>2</sub> and Ar to quantify net biological production of oxygen, while correcting for physical processes. Both gases are affected by physical processes such as gas exchange, but O<sub>2</sub> is also produced by photosynthesis and consumed by respiration. Thus, the ratio of the two gases quantifies the relative amount of O<sub>2</sub> produced by biological activity, a measure of NCP. This method has been used since the late 1980s with great success to constrain rates of NCP (~~Bender et al. 1999, Cassar et al. 2007, Craig & Hayward 1987, Emerson et al. 1991, Hendricks et al. 2004, Hendricks et al. 2005, Juranek & Quay 2005, Juranek & Quay 2010, Juranek et al. 2012, Quay et al. 2010, Reuer et al. 2007, Spitzer & Jenkins 1989~~)(Bender et al. 1999, Cassar et al. 2007, Craig & Hayward 1987, Emerson et al. 1991, Hendricks et al. 2004, Hendricks et al. 2005, Juranek & Quay 2005, Juranek & Quay 2010, Juranek et al. 2012, Quay et al. 2010, Reuer et al. 2007, Spitzer & Jenkins 1989). A recent advance is the development of an at-sea mass spectrometer that allows continuous measurement of O<sub>2</sub>/Ar from the underway system of a ship (~~Cassar et al. 2009, Hamme et al. 2012, Lockwood et al. 2012, Stanley et al. 2010~~)(Cassar et al. 2009, Hamme et al. 2012, Lockwood et al. 2012, Stanley et al. 2010).

In order to calculate NCP from O<sub>2</sub>/Ar records, steady state is often assumed and NCP is calculated by an assumed balance between biological production and gas exchange (e.g., ~~Reuer et al. 2007~~)(e.g., Reuer et al. 2007). In SMS frontal regions, however, a steady state assumption may not be valid. Additionally, physical transport of waters with varying O<sub>2</sub>/Ar becomes more critical in frontal regions since vertical velocities are enhanced at fronts (~~Klein & Lapeyre 2009, Legal et al. 2007~~)(Klein & Lapeyre 2009, Legal et al. 2007). However, by tracking a patch of water in a Lagrangian sense, as we are proposing to do here with the model solution, and eventually with observations, ***we do not need to assume steady state***. Instead, we will directly calculate the rate of change of O<sub>2</sub>/Ar as we follow the patch. This non-steady state method has been used successfully in the Southern Ocean to calculate rates of NCP (~~Hamme et al. 2012~~)(Hamme et al. 2012). An advantage of this non-steady state approach is that O<sub>2</sub>/Ar is reflecting “real-time” productivity, i.e. ***reflecting changes in productivity over time-scales of approximately a day***. This is in contrast to the time scales of one to two weeks that is typical when using the steady-state assumption.

Additionally, we will estimate the effects of vertical and horizontal mixing on the O<sub>2</sub>/Ar. In particular, we will add an Ar tracer to the LOBSTER model. This will allow direct testing of the assumptions that go into calculating NCP from O<sub>2</sub>/Ar; and 2) enable the synthesis of the NCP rates with the physical framework. O<sub>2</sub> and Ar have been used in other models to look at the validity of the assumptions usually made when calculating NCP (~~Jonsson et al. 2013~~)(Jonsson et al. 2013) but not yet at submesoscales. -We will also estimate the effects of vertical mixing by combining canonical estimates of diapycnal diffusivity with gradients of O<sub>2</sub> calculated from O<sub>2</sub> profiles collected at spatial resolution of approximately 1.5 km in the upper 150 m from the VPR (~~Davis et al. 2005~~)(Davis et al. 2005). Mixed layer depth can be calculated from VPR and MVP data, and thus we can calculate changes in O<sub>2</sub> that are a result of entrainment from water below the mixed layer (~~Jonsson et al. 2013~~)(Jonsson et al. 2013). To estimate effects of lateral transport, we will use O<sub>2</sub>/Ar determined in the spatial survey when we are first mapping out a feature. In past studies, the effects of vertical and lateral mixing have been small compared to the production terms and we expect the same here (Hamme et al. 2012).

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Of course, the primary objective of the EXPORTS program is to determine the fate of NCP, and thus the bulk of our OSSE work will be focused on that aspect. Again, simulated data will be collected from the wide variety of sampling platforms to be deployed (Figure 11), thus allowing us to evaluate the degree to which the various pathways of export will be quantified by the proposed measurement program. A particularly interesting aspect in this regard is export via submesoscale subduction, which in some cases may be as large as or larger than that brought about by sinking particulate matter (Omand et al. 2015). Finally, we intend to use our results to evaluate various methods for inferring export production from satellite data (e.g. Laws et al. 2011, Nevison et al. 2012, Siegel et al. 2014); a recent study by Stukel et al. (2015) provides an observational assessment using Lagrangian-based process studies.

## 5. Project management and timeline

As lead PI of the project, Dr. McGillicuddy will oversee all aspects of the proposed research. Most of the hands-on modeling work will be carried out by Dr. Valery Kosnyrev, a ~~graduate student~~ Research Associate in the MIT/WHOI Joint Program. ~~Dr. McGillicuddy's laboratory.~~ Dr. McGillicuddy will work closely with Dr. Lévy in supervising ~~the student~~ Dr. Kosnyrev's work, and this collaborative effort will involve yearly visits to Dr. Lévy's laboratory. The first such visit will be ~~three months~~ two weeks in duration ~~for the student (two weeks for to allow Dr. McGillicuddy) to allow sufficient time for learning to become familiar with running the LOBSTER-oxv model and incorporating oxygen dynamics into the code.~~ Thereafter, the visits will be shortened to one ~~month per year for the student, and one week per year for Dr. McGillicuddy.~~ We expect two and Lévy to participate in joint analysis and interpretation of these visits will be coordinated with SWOT science team meetings held in Europe, thereby defraying travel expenses. ~~the results.~~

<u>Workplan and Key Milestones</u>	<u>Yr 1</u>	<u>Yr 2</u>	<u>Yr 3</u>
<u>1) Test oxygen dynamics in LOBSTER model</u>	<u>2</u>		
	<u>2*</u>		
	<u>10</u>		
<u>2) Carry out high-resolution simulations</u>	<u>1</u>	<u>1</u>	
	<u>1*</u>	<u>1</u>	
	<u>25</u>	<u>15</u>	
<u>3) Compare simulated and observed hotspots</u>	<u>10</u>	<u>5</u>	
	<u>7*</u>	<u>4</u>	
	<u>15</u>	<u>10</u>	
<u>4) Revise the biogeochemical model</u>		<u>7</u>	
		<u>5</u>	
		<u>25</u>	
<u>5) Simulate sampling of hotspots by remote sensing: altimetry, SST, ocean color</u>			<u>3</u>
			<u>2.5</u>
			<u>15</u>
<u>6) Evaluate the accuracy of hotspot reconstruction</u>			<u>3</u>
			<u>2.5</u>
			<u>15</u>
<u>7) Carry out OSSEs for in situ process studies</u>			<u>7</u>
			<u>5</u>

The work plan milestones are summarized in the table below. Drs. McGillicuddy and Lévy's effort are allocated to each task in proportion to the time. In year 1, the student Dr. Kosnyrev will learn the LOBSTER configuration model and with BATS data (Objective 1). That will

			20
<b>Totals</b>			
McGillicuddy	13	13	13
Lévy	10*	10*	10*
Kosnyrev	50	50	50
Barkley	4	4	4
<i>Project timeline. Allocation of effort for the two scientific investigators (McGillicuddy, Lévy), Research Associate Valery Kosnyrev, and an administrative professional (Barkley) is indicated as a percent of full time. Ms. Barkley will provide administrative assistance with annual reports, budget tracking, manuscript preparation, travel, and other administrative tasks. Asterisks indicate that Dr. Lévy's time will be covered by her ongoing grants and internal support from UPMC.</i>			

and key below. Lévy's each task student's start by model testing it take with the

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approximately half time, balance spent on. Once that is completed, he will begin carrying out the initial high-resolution simulations (Objective 2). That activity) and comparing the simulated hotspots with observations (Objective 3). These activities will continue into year 2, when the simulated and observed hotspots will be compared in detail (Objective 3). That will set the stage for any needed revisions to the biogeochemical model are implemented (Objective 4), estimated to be an approximately 50 percent effort in year 2. We expect that model revision and comparison with observations will be an iterative process that will continue into year 3. Once the simulations are finalized, we will begin simulating sampling of hotspots by SWOT and other various remote sensing platforms (Objective 5). That activity will continue into year 4 as we, which will allow us to evaluate the accuracy with which hotspots can be reconstructed from satellite data alone (Objective 6). Lastly, we will carry out OSSEs for *in situ* process studies that will maximize the scientific utility of SWOT for coupled physical-biological-biogeochemical investigations of this type inform the EXPORTS field program in the North Atlantic (Objective 7).

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— We note that as an international collaborator, Dr. Lévy is not requesting any salary support from NASA. The percent effort reported in the table below reflects that which she can allocate as part of her academic appointment as well as synergy with ongoing research projects (indicated with an asterisk below).

Workplan and Key Milestones	Year 1	Year 2	Year 3	Year 4
1) Incorporate oxygen dynamics	4			
	5*			
	50			
2) Carry out high-resolution simulations	4	2.5	2.5	
	5*	2.5*	2.5*	
	50	25	25	
3) Compare simulated and observed hotspots		2.5	2.5	
		2.5*	2.5*	
		25	25	
4) Revise the biogeochemical model		5	5	
		5*	2.5*	

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		50	25	
5) Simulate sampling of hotspots by SWOT and other sensors			2.5	3.125
			2.5*	2.5*
			25	25
6) Evaluate the accuracy of hotspot reconstruction				3.125
				2.5*
				25
7) Carry out OSSEs for <i>in situ</i> process studies				6.25
				5*
				50
Totals				
McGillicuddy	8	40	42.5	42.5
Lévy	40*	40*	40*	40*
Graduate Student	100	100	100	100
Barkley	4	4	4	4

*Project timeline.* Allocation of effort for the two scientific investigators (McGillicuddy, Lévy), MIT/WHOI Joint Program Student, and an administrative professional (Barkley) is indicated as a percent of full time. Ms. Barkley will provide administrative assistance with annual reports, budget tracking, manuscript preparation, travel, and other administrative tasks.

## 6. Data management and sharing plan

We recognize that the proposed data products and simulations will contain phenomenological richness that cannot be fully exploited by a single research group over the course of one grant. As such, it is very important to us to make our results available to the broader scientific community. We will develop and maintain a project web site on which the data products and model solutions will be archived at suitable space/time resolution for others to use in their own investigations. This archive will be served from our in-house RAID array. Moreover, we will serve the codes specific to our implementation of the LOBSTER model, subsampling tools, and associated analysis software (e.g. Matlab and Fortran 90 scripts). The project archive should thus provide potential users with everything they need to interrogate our data products and model solutions for a particular process in which they are interested. We hope that the availability of these materials will help nurture additional comparisons between observations and models, as well as further refinement of coupled physical-biological-biogeochemical models themselves.

## 7. Perceived impact and relevance to the SWOT science team ~~NNH15ZDA001N-OB~~

The impact of this effort stems from our interdisciplinary approach to remote sensing, using data collected with advanced observational techniques, and integrated analysis in the context of a state-of-the-art coupled physical-biogeochemical model. ~~This combination of observations and modeling will facilitate testing of the hypothesis  $H_0$ : Submesoscale nutrient injections stimulate phytoplankton production, increasing NCP rates. The proposed Observing System Simulation Experiments will set the stage for definitive observational testing of these ideas once the SWOT mission becomes operational. Carrying out such OSSEs in advance will lend confidence that the sampling strategy will be capable of resolving the SMS features of interest—an issue that has posed a major challenge to past efforts.~~

The proposed research incorporates multiple satellite missions together with *in situ* data and numerical models to improve our understanding of physical-biological interactions at the

mesoscale and submesoscale. ~~As such, it resonates with theme 2.2 of solicitation NNH11ZDA001N, Mesoscale and Submesoscale processes: “Both modeling and observational studies will be needed to develop ideas and methodologies to maximize the science return of SWOT observations.”~~ Although our focus is not solely on physical oceanography and circulation per se, satellite altimetry provides the foundation for this activity. As such, we submit that the SWOT science team is an ideal environment for this interdisciplinary research. Lastly, we note that the research proposed herein on submesoscale dynamics is entirely complementary to Dr. McGillicuddy’s contribution to the Ocean Surface Topography Science Team (OSTST), which focuses squarely on mesoscale (results reported in Dr. McGillicuddy’s Biographical Sketch). This will improve our knowledge of the mechanistic links between physical forcing, upper ocean chlorophyll distributions, and biogeochemical cycling. Such synthesis will lead to better quantification of carbon fluxes throughout the global ocean, and the processes by which those fluxes may respond to climate variability and change.

The proposed research is relevant to theme 2.2 of solicitation NNH15ZDA001N-OBB, “Global Data Sets and Modeling In Support of Planned Northeast Pacific and North Atlantic Export Flux Studies.” Specifically, we will conduct Observing System Simulation Experiments in support of the EXPORTS field campaign in the North Atlantic. These will be completed in year 3 of the project, which will allow sufficient time for the results to inform execution of the seagoing campaign planned for 2020. Although our results will obviously not impact the sampling strategy for the Northeast Pacific field work, we expect that our findings will aid the analysis and synthesis of those results from a process-oriented point of view.

Lastly, we note that the proposed international collaboration between the laboratories of Drs. McGillicuddy and Lévy fits within the emerging framework for coordinated studies of the Atlantic, as described in the trilateral Galway Statement on Atlantic Ocean Cooperation<sup>3</sup> among the European Union, Canada, and the United States.

## 8. Computational resources

In year one, we will test the implementation of LOBSTER-oxy at coarse resolution (ca. 1.0°), which will be perfectly feasible on desktop workstations available in the laboratories of Drs. McGillicuddy and Lévy. Initial high-resolution simulations of limited duration will be carried out on WHOI’s linux cluster “Scylla”. As we proceed with production runs ~~in year 2~~, we expect to make a request for NASA High-End Computing (HEC). We estimate that the high-resolution runs will require approximately the same amount of resources as the 0.1° resolution global simulations that have been supported by ongoing HEC grants to Dr. McGillicuddy (Group ID s0847) as part of the OSTST, amounting to ca. 1,000,000 processor-hours (ca. 87,000 SBUs).

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<sup>3</sup> <http://www.coopeus.eu/galway-statement/>

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## Statements of Commitment

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Subject: ~~letter of Commitment~~  
Date: ~~Wed, 6 May 2015 10:46:11 +0200~~  
From: ~~Marina Lévy <marina@locean-ipsl.upmc.fr>~~  
To: ~~Dennis McGillicuddy <megillie@whoi.edu>~~  
CC: ~~Marina Lévy <Marina.Levy@locean-ipsl.upmc.fr>~~

### Letter of Commitment

I acknowledge that I am identified by name as Co-Investigator to the investigation entitled “Mesoscale and submesoscale physical-biological interactions: will the SWOT altimeter resolve the mechanisms controlling hotspots in net community production?”, that is submitted by Dennis J. McGillicuddy, Jr. to the NASA Research Announcement NNH15ZDA001N-SWOT, and that I intend to carry out all responsibilities identified for me in this proposal. I understand that the extent and justification of my participation as stated in this proposal will be considered during peer review in determining in part the merits of this proposal. I have read the entire proposal, including the management plan and budget, and I agree that the proposal correctly describes my commitment to the proposed investigation.

Sincerely,

~~/Marina Lévy/  
/LOCEAN IPSL //~~  
~~/Tel: +33 (0)1 44 27 27 07/~~  
~~/UPMC, Tour 45, 4eme, BC 100 /~~  
~~/skype id: marina.levy/~~  
~~/4 Place Jussieu, F 75252 Paris Cedex 05 /~~  
~~/http://www.locean-ipsl.upmc.fr/~marina/~~

~~Subject: Letter of Commitment~~  
~~Date: Wed, 06 May 2015 13:29:38 -0400~~  
~~From: Valery Kosnyrev~~  
~~Shirley Barkley <sbarkley@whoi.edu>~~  
~~To: McGillicuddy, Dennis <dmcgillicuddy@whoi.edu>~~

~~Letter of Commitment~~

~~I acknowledge that I am identified by name as Co-Investigator to the investigation entitled "Mesoscale and submesoscale physical-biological interactions: will the SWOT altimeter resolve the mechanisms controlling hotspots in net community production?", that is submitted by Dennis J. McGillicuddy, Jr. to the NASA Research Announcement NNH15ZDA001N-SWOT, and that I intend to carry out all responsibilities identified for me in this proposal. I understand that the extent and justification of my participation as stated in this proposal will be considered during peer review in determining in part the merits of this proposal. I have read the entire proposal, including the management plan and budget, and I agree that the proposal correctly describes my commitment to the proposed investigation.~~

~~Sincerely,  
Shirley Barkley  
Applied Ocean Physics & Engineering  
Woods Hole Oceanographic Institution  
Woods Hole, MA 02543~~

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## **Budget ~~Justification~~Information**

The Woods Hole Oceanographic Institution (WHOI) is a non-profit [501c(3)] research and education organization subject to the cost principles of 2 CFR ~~230.200~~. WHOI Principal Investigators are responsible for conceiving, funding and carrying out their research programs. ~~Many of them also constitute the educational faculty of the Institution.~~ Senior Personnel are expected to raise 12 months of support for themselves and their staff by writing proposals and obtaining sponsored research grants and contracts from a variety of sources. ~~Those who participate~~ Some teach voluntarily in ~~WHOI's academic programs receive an average of only 2 months of Institution~~ MIT/WHOI's Joint Program, but support ~~per calendar year, and participation in teaching and advising for this is neither required nor universal.~~ NSF has confirmed to WHOI that salary support beyond 2 months per year can be justifiable in grants for ~~these~~ WHOI Principal Investigators.

The rates included in the proposal are negotiated with our cognizant government agency (Office of Naval Research).

For 2016 proposed costs, WHOI calculates overhead rates (both Laboratory Costs and General & Administrative Costs) as a percent of total direct salaries and benefits, as allowed by 2 CFR ~~230.200~~. Direct salaries exclude overtime-premium pay.- A proposed labor month is equal to 152 hours or 1824 hours annually versus 2080 hours (40 hours/week for 52 weeks). -The difference is for vacations, holidays, sick time, and other paid absences, which are included in the Paid Absences calculation. \_ WHOI cannot "waive" or reduce overhead rates on any sponsored research project due to the structure of our negotiated rates with our cognizant government agency.-\_ When a program sets limits on overhead, WHOI must use Institution unrestricted funds to pay the unfunded portion of the overhead costs.

~~Graduate student stipends are included in the total direct salary costs. However, they are not included in the benefits base, and only 1/2 of the Laboratory Cost rate is applied to the stipend because it is estimated that the GRA occupies a laboratory only 1/2 of his/her time, and the balance is spent in education activities. Fifty five percent (55%) of the GRAs' tuition is included as a direct cost in this budget. The Institution provides the balance from Institution endowment funds, including 100% of summer tuition.~~

~~The rates included in the proposal are negotiated with our cognizant government agency or they are estimates. When estimated rates are finalized, costs will be in accordance with the rate agreement.~~

In December 2015 WHOI received approval from our cognizant government agency to change the method of allocation of indirect costs to Modified Total Direct Costs (MTDC) effective 1/1/2017. Therefore, for 2017 and beyond, the MTDC allocation method is used to calculate indirect costs. The normal exclusions contained in 2 CFR 200.68 (MTDC) apply, as well as the following approved exclusions: ship use, submersible use, vessel charters and ship fuel.

Due to the change in WHOI's method of allocation of indirect costs to MTDC beginning January of 2017, any period of performance that crosses between calendar years 2016 and 2017 requires

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the budget to be broken out by calendar months and what effort is in 2016 vs. 2017, as we cannot use two different methods to allocate indirect costs in one period.

### **Budget justification**

As lead PI of the project, Dr. McGillicuddy will oversee all aspects of the proposed research. ~~Most of the~~ The hands-on modeling work will be carried out by ~~a graduate student in the MIT/WHOI Joint Program.~~ Dr. Valery Kosnyrev, a Research Associate III who has worked in Dr. McGillicuddy's laboratory for more than 15 years. Dr. McGillicuddy will work closely with Dr. Lévy in supervising ~~the student~~ Dr. Kosnyrev, and this collaborative effort will involve yearly visits to Dr. Lévy's laboratory (see below). ~~We note~~

Note that a student ideally suited to the proposed research was recently admitted to the MIT/WHOI Joint Program. She has indicated her intention to matriculate this coming fall, and is considering Dr. McGillicuddy as a potential supervisor. If, in the event the student decides to choose another supervisor, we would seek to renegotiate this the year 1 budget line for a Research Associate III in Dr. McGillicuddy's lab to carry out those tasks is split into two periods, as required by the change in accounting for indirect costs that will take place 1 January 2017 (see above).

The work plan and key milestones are summarized in the table below. Drs. ~~McGillicuddy and Lévy's effort are allocated to each task in proportion to the student's time. Dr. McGillicuddy's salary request increases over the course of the project (1.0, 1.25,~~ McGillicuddy and Kosnyrev require 1.5; and 1.56 months of salary per year in years 1-4, respectively), owing to the ~~increasing effort he will allocate to synthesis and publication of the results (although the graduate student will likely be the lead author on most of the resulting publications). We note that as order to carry out the proposed research. As~~ an international collaborator, Dr. Lévy is not requesting any salary support from NASA. The percent effort reported in the table below reflects that which she can allocate as part of her academic appointment as well as synergy with ongoing research projects ~~(indicated by an asterisk below).~~

In year 1, ~~the student~~ Dr. Kosnyrev will start by learning the LOBSTER model and enhancing it to the LOBSTER-oxy configuration model and testing it with BATS data (Objective 1). ~~That will take approximately half time, with the balance spent on~~ Once that is completed, he will begin carrying out the initial high-resolution simulations (Objective 2). ~~That activity~~ and comparing the simulated hotspots with observations (Objective 3). These activities will continue into year 2, when ~~the simulated and observed hotspots will be compared in detail~~ (Objective 3). ~~That will set the stage for~~ any needed revisions to the biogeochemical model ~~are implemented~~ (Objective 4), ~~estimated to be an approximately 50 percent effort in year 2.~~ We expect that model revision and comparison with observations will be an iterative process that will continue into year 3-). Once the simulations are finalized, we will begin simulating sampling of hotspots by SWOT and ~~other various~~ remote sensing platforms (Objective 5). ~~That activity will continue into year 4 as we), which will allow us to~~ evaluate the accuracy with which hotspots can be reconstructed from satellite data alone (Objective 6). Lastly, we will carry out OSSEs for *in situ* process studies that will ~~maximize the scientific utility of SWOT for coupled physical-biological-biogeochemical investigations of this type~~ inform the EXPORTS field program in the North Atlantic (Objective 7).

Two weeks of administrative assistance (S. Barkley) will be required each year to assist with annual reports, budget tracking, manuscript preparation, travel, and other administrative tasks.

Fringe: Fringe Benefits at WHOI are calculated at ~~40.93~~ 37.00% as negotiated with our cognizant government agency. Total fringe requested for WHOI employees as part of this proposal is \$~~142,377 [31,867~~ 83,323 [26,826/Y1; ~~44,004~~ 27,762/Y2; ~~32,601~~ 28,735/Y3; ~~33,905/Y4~~].

Workplan and Key Milestones	Yr 1	Yr 2	Yr 3
1) Test oxygen dynamics in LOBSTER model	2		
	2*		
	10		
2) Carry out high-resolution simulations	1	1	
	1*	1	
	25	15	
3) Compare simulated and observed hotspots	10	5	
	7*	4	
	15	10	
4) Revise the biogeochemical model		7	
		5	
		25	
5) Simulate sampling of hotspots by remote sensing: altimetry, SST, ocean color			3
			2.5
			15
6) Evaluate the accuracy of hotspot reconstruction			3
			2.5
			15
7) Carry out OSSEs for <i>in situ</i> process studies			7
			5
			20
Totals			
McGillicuddy	13	13	13
Lévy	10*	10*	10*
Kosnyrev	50	50	50
Barkley	4	4	4
<i>Project timeline. Allocation of effort for the two scientific investigators (McGillicuddy, Lévy). Research Associate Valery Kosnyrev, and an administrative professional (Barkley) is indicated as a percent of full time. Ms. Barkley will provide administrative assistance with annual reports, budget tracking, manuscript preparation, travel, and other administrative tasks. Asterisks indicate that Dr. Lévy's time will be covered by her ongoing grants and internal support from UPMC.</i>			

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We request travel support for Dr. McGillicuddy ~~and the graduate student~~ to visit Dr. Lévy's laboratory in Paris. The first such visit will be ~~three months~~two weeks in duration ~~for the student (two weeks for Dr. McGillicuddy)~~ to allow sufficient time for learning the LOBSTER model ~~and incorporating oxygen dynamics into the code.~~ Thereafter, the visits will be shortened to one month per year for the student, and one week per year for Dr. McGillicuddy. ~~Two of these visits will be coordinated with SWOT science team meetings held in Europe (years 2 and 4), which will defray travel expenses.~~

We request travel support each year for Dr. McGillicuddy ~~and the graduate student~~ to attend yearly meetings of the ~~SWOT Science~~Ocean Color Research Team, ~~alternating between San Diego, CA (years 1 and 3) and Toulouse France (years 2 and 4).~~ The yearly request includes airfare, ground transportation, and per diem for ~~5 days~~ for each traveler; assuming the meeting will take place on the West Coast, we have used San Diego as a point of destination. Estimates for airfare are based on rates currently available on Expedia/~~American Express~~ for refundable tickets and include an allowance for baggage and agent fees. Ground transportation costs include rental car(s) and transportation to/from the airports. Per diem expenses are based on rates currently available via the GSA website (<http://www.gsa.gov/portal/category/21287/content/104877>) for domestic travel and [https://aoprals.state.gov/content.asp?content\\_id=184&menu\\_id=78](https://aoprals.state.gov/content.asp?content_id=184&menu_id=78) for foreign travel. All rates are increased by 10% in subsequent years to account for rate hikes. ~~In years 2 and 4, travel to the SWOT science team meetings will be combined with visits to Dr. Levy's laboratory in Paris in order to save on travel expenses.~~

~~Standard laboratory operations will require computer supplies (toner cartridges, paper, and electronic storage devices) in all four years. Cost estimates are based on previous purchases of a similar nature.~~

~~Publication costs are requested in years 2-4 to cover dissemination of the scientific results in peer-reviewed journals. These costs include color figures (\$400 per year) and 8 hours of graphic shop services (hourly rates of \$83, \$84, \$85) and page charges (\$1875, \$1950, \$2025) each year.~~

~~Communication costs are requested each year to cover phone calls and faxes between PI and program manager, collaborators and vendors. A small amount is requested for Shipping and Postage costs each year. Cost estimates are based on previous purchases of a similar nature.~~

~~Facilities and computer maintenance:~~ The network of workstations and servers currently available in Dr. McGillicuddy's laboratory will be sufficient for the proposed research. However, the computational infrastructure in Dr. McGillicuddy's laboratory must be kept current. Five thousand dollars per year ~~are~~is requested in computer supplies for CPU upgrades, additional disks, backup units, and other items needed to maintain the ~~local facilities~~computer systems we will be using in this research. Cost estimates are based on previous purchases of a similar nature.

Publication costs are requested in years 2 and 3 to cover dissemination of the scientific results in peer-reviewed journals. These costs include color figures (\$400 per year) and 8 hours of graphic shop services (hourly rate of \$85) and page charges (\$1920) each year.

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Communication costs are requested \$200 each year to cover phone calls and faxes between PI and program manager, collaborators and vendors. Cost estimates are based on previous purchases of a similar nature.

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Workplan and Key Milestones	Year 1	Year 2	Year 3	Year 4
1) Incorporate oxygen dynamics	4			
	5*			
	50			
2) Carry out high-resolution simulations	4	2.5	2.5	
	5*	2.5*	2.5*	
	50	25	25	
3) Compare simulated and observed hotspots		2.5	2.5	
		2.5*	2.5*	
		25	25	
4) Revise the biogeochemical model		5	5	
		5*	2.5*	
		50	25	
5) Simulate sampling of hotspots by SWOT and other sensors			2.5	3.125
			2.5*	2.5*
			25	25
6) Evaluate the accuracy of hotspot reconstruction				3.125
				2.5*
				25
7) Carry out OSSEs for <i>in situ</i> process studies				6.25
				5*
				50
Totals				
McGillicuddy	8	40	42.5	42.5
Lévy	40*	40*	40*	40*
Graduate Student	400	400	400	400
Barkley	4	4	4	4

Project timeline. Allocation of effort for the two scientific investigators (McGillicuddy, Lévy), MIT/WHOI Joint Program Student, and an administrative professional (Barkley) is indicated as a percent of full time. Ms. Barkley will provide administrative assistance with annual reports, budget tracking, manuscript preparation, travel, and other administrative tasks.