## **Reply comments Referee #2:**

This paper relies on the spatio-temporal variability of the HNLC regions identified by SOM over the three major ocean areas using satellite-derived chlorophyll-a and modeling outputs of nutrients. The authors have performed the NO3:Chl as an indicator of the distribution limit of HNLC. They have demonstrated the linkages between HNLC extent and some climate-driven factors and teleconnections.

As a first very general comment, I would say that this is a valuable case study that can be published with some major corrections. The authors presented a lot of data and analysis procedures that need accurate processing schemas and precise interpretation, which they handled well.

The introduction section is well written and presents an adequate understanding of the presented work. The methodologies are adequate, but need some improvements. Some supplementary materials may be inserted into the main text because of their essential investigations and frequent references to them (e.g., Fig. S2).

## We are grateful for the generally positive review of RC2. We have improved some aspects of the M&M section and a figure from supplementary material is now included in the main text as Fig.1

The Spatio-temporal variability of HNCL/NO3:Chl should be presented more precisely and quantitatively. For example, maps of monthly climatology, charts and maps of inter-annual cycles, and spatial-temporal cross section such as Hovemoler chart may present valuable results.

The aim of the SOM analysis is precisely to replace this type of traditional climatology analysis with more objective, quantitative, and precise approaches. SOM analysis allows the reconstruction of the spatial patterns and their temporal dynamics (seasonal and interannual) of the study variables (i.e. using the results shown in Figures 4, 5, and 6). The SOM mapping has advantages over other methodologies, e.g. monthly climatology, maps of inter-annual cycles), as relevant time and spatial scales are unveiled without any prefixed assumption. For instance, if two different spatial patterns occur in the same month with the same probability, using a monthly average only one spatial pattern will be obtained, while SOM should identify both patterns. We explain this more profusely now.

Some of the findings of the results section have not been well demonstrated in this study (e.g., section 3.4.1 Influence of SST variations – the global power spectra of CWT are needed to explain the intra-annual and inter-annual cycles). Some contents of Figures need to be better framed/explained. Some words would be expressed in accurate form. e.g., it is not clear in many places in the text that the "wind" word is mean wind speed, or wind vectors, or wind stress, or wind components (zonal and meridional).

We have removed the section explaining variations in SST because it is not a forcing. The term wind has been reviewed throughout the document and, particularly in section 4.2, and we specify now whether we refer to wind intensity, etc..

I think a discussion section is required to explain the performance and limitations of the presented methodologies and results, which are not seen in this manuscript.

Following the reviewer's suggestion, we have reformatted the results and discussion section into separate sections and we further discuss the presented methodologies.

Bioregionalization analysis was used in previous studies to classify the global oceans (e.g., Longhurst, A. (2007), Ecological Geography of the Sea, Academic Press, London). Could the author highlight the need to new ocean's regionalization which are not accessible from available global regionalization? And why SOM and not the other classification methods such as k-means?

Bioregionalizations can be based on different variables and generally differ in that they obey different requirements. It is simply not possible to analyze certain environmental issues from regionalizations based on low-resolution information or criteria that do not respond to the object of the study. This is particularly true in the case of the study of pelagic organisms where the biome extent changes over time. The first regionalizations proposed by Alan Longhurst (1995 and 1998) obeyed geographic divisions based on the average distribution of phytoplankton biomass and primary production and provided a coarse but useful division of the global ocean. In subsequent analyses, other components of the trophic chains were incorporated. In specific cases such as HNLC, the biome presents highly dynamic boundaries and it becomes necessary to resort to techniques that incorporate this variability.

Self-Organizing Maps (SOM) and k-means are both unsupervised machine learning algorithms, but they have different characteristics and are used for different purposes. K-means is a clustering algorithm that groups similar data points together based on spherical clusters, while SOM finds the best matching unit (BMU) for each data point, which is the node in the grid that is most similar to the data point. Also, SOMs can handle non-linearly separable data.

One of the advantages of the SOM over k-means is that it performs the groupings based on the shape of the time series, which provides very coherent regions with similar dynamics, which allows each subregion to be characterized later based on robust statistics.

The SOM non-linear mapping has also advantages over linear methodologies, like principal component analysis, empirical orthogonal functions (EOF), and even K-means. If the data distribution on a two-dimensional space has a correlation close to zero, this can be difficult to find it using PCA or similar, however, by using SOM, the resulting weights will be adjusted in such a way as to match the shape of the data distribution. K-means is a special case of SOPM in which the neighborhood function is zero (not considered).

I think the findings of the nutrient model are not presented well. Some additional information is required.

We do not run a nutrient model. Results are from the numerical simulation PISCES produced at Mercator-Ocean (https://www.pisces-community.org/ https://www.pisces-community.org/index.php/model-description/). It runs over NEMO hydrodynamic model, a primitive equations model https://www.nemo-ocean.eu/ and therefore, it does consider MLD. However, we did compare model results with available data globally and regionally and we provide now the correlations between model data and regional data for global and regional data. We also include now in the supplementary information the mean NO3 profile in each region depicted from in situ data,

The Mixed Layer Depth (MLD) is one of the main oceanographic indicators that can be used for the interpretation of nutrients and phytoplankton variabilities. Does the nutrient

model consider the MLD? If yes, please indicate in the text. And if not, I think it is required to consider the global ocean MLD in your work.

## Yes, it considers the MLD. Answered above

Looking to be constructive, in addition to the overall comments above, which should be taken into account in a possible review, I would like to point out the following Remarks.

1- In the 2.1 Ocean color data:

The GlobColour data are presented in 25 km spatial resolution globally. The authors have mentioned that the composites have a  $0.25^{\circ}$  spatial resolution. We know that the spatial resolution of 25 km and  $0.25^{\circ}$  are not the same specially at higher latitudes. If the  $0.25^{\circ}$  is true, please explain the spatial interpolation methods. If not, please correct.

The reviewer makes a good point here. The GlobColour level-3 mapped products have a resolution of 1/24°, 0.25° or 1.0° (i.e. respectively around 4.63 km, 28 km, and 111 km at the equator) for global products. They consist of the flux-conserving resampling of the global level-3 binned products. The geographical location and extent of each bin is determined by the so-called Integerized Sinusoidal (ISIN) grid. In particular, we use data from the rectangular regular map product provided by GOBCOLOUR at global scale, with a regular grid in degrees, with a spatial resolution of 0.25 degrees, 27.82km at the equator that varies with the latitude. The spatial extent was given in pixels and it has been changed to 'real' areas in km2 in this new version. Data are not interpolated since they are structured in a regular grid.

As a result of these changes, small variations are observed in the mean climatology of the area anomaly for the three HNLC regions. Intra and interannual area variations in EEP and SNP regions are slightly larger when computing the area based on the linear dimension (i.e. km<sup>2</sup>) than on the number of pixels.

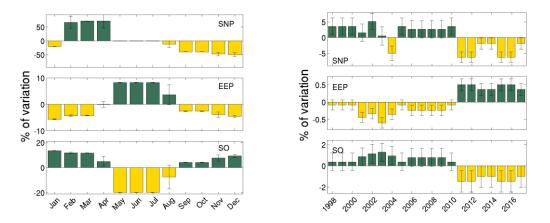


Figure R1. Seasonal (left) and interannual variations (right) in the spatial extension of the three HNLC regions. Variations are referred to the mean extension of each region. The blue dashed lines indicate the regime shift occurring after 2010.

2- In the section: 2.2 Nitrate data the authors have made some essential assumptions that need to be approved precisely. May be explain more in the Results.

We now explain better matching between model and in situ values in each HNLC region. We also include nutrient profiles in the supplementary information.

3- Please provide more information about the setup of the SOM algorithm (which are available not in the text nor supplementary material), in particular about the initial configuration: linear or random initialization, sheet or toroidal network, etc. Which neighbor function (Gaussian, Ep, et) is used to update the neighbors of the excited neuron (BMU) after each iteration during the training process.? Did the authors check the sensitivity of the SOM pattern to linear and random initialization?

The SOM algorithm is composed of two main steps: initialization and training. In the initialization, the architecture of the neural network used in this study is set in a sheet hexagonal map lattice of neurons, or units, in order to have equidistant neurons (to avoid anisotropy artifacts). Each unit is represented by a weight vector with a number of components equal to the dimension of the input data, i. e. number of rows or number of columns in the Chl and NO3 matrices, depending on whether the analysis is performed in the temporal or in the spatial domain. We use an initial network composed of units of random values (random initialization). In the training process, the initial neural network is transformed by iteratively presenting the input data. In each successive iteration the neuron, or unit, with the greatest similarity (excited neuron), called Best Matching Unit (BMU) is updated by replacing their values with the Chl and NO3 values of the input sample data. The similarity is estimated by computing the Euclidean distance between the components of the input sample and the components of the weight vector of the unit. The unit most similar to the input sample is the one with the minimum distance. In the learning process, Chl and NO3 values of the neighboring neurons of the excited neuron are also updated replacing their values with values determined by a neighborhood function. In this way, the topological neighbors of the BMU are also updated through the neighborhood function. In this study, we use the imputation batch training algorithm (Vatanen et al., 2015) and a Gaussian neighboring function. We do not find important differences between linear and random initialization. However, linear initialization is more computationally expensive.

4- The output of the SOM is also not well defined beyond being a map or topology; for example, how are the errors computed? The number of neurons is chosen not only depending on the topological errors (or topographic errors), but also on quantization errors. How different are the patterns when the number of neurons is, for example, 9?

The size of the neural network (number of neurons) depends on the number of samples and on the complexity of the patterns and an optimal choice is important to maximize the quality of the SOM. In the present study, the map size is set to be  $[4 \times 3]$  with 12 neurons for the time domain analysis, and a  $[3 \times 3]$  neural network is used in the spatial domain. Using larger map sizes, the patterns are slightly more detailed, and more regions of a particular variability emerge, but the occurrence of the probability of the patterns decreases, without affecting the results noticeably (Basterretxea et al., 2018; Hernandez-Carrasco and Orfila, 2018). If a reduced neural map, such as  $[2 \times 2]$  is used, patterns are concentrated together with the occurrence probability in a few rough patterns but increasing, in this case, the topological error. 5- Figure 6 and 7. The arrows are too small.

This has been corrected.

6- I recommend to show the time-series anomaly of HNLC and teleconnections at the top of the Fig. 6 and indicate the significant inter-annual cycles.

Figure 6 has been removed following a reviewers suggestion

7- It is hard for readers to infer the shift after 2010 (Fig. 5). I think more visualization/explanations of data are required.

We indicate the shift with a blue dashed line in the figure.

8- There are some abruptions in the significant annual cycles (1.5 year, from year 2006 to 2010) in the Fig. 7 which need to be explained. I suggest perform the global spectral cycles graphs.

We have improved the figure including mean spectral peaks and further explanation is provided.

9- The authors have considered SST and the teleconnections as a factor controlling HNLC variability. Are there any environmental factors such as precipitation and wind stress that may affect HNLC variability? Please discuss.

We have segregated results from discussion and a more detailed discussion on teleconnections is now provided. This includes ENSO associated effects. However, the analysis of particular factors, such as rainfall, is beyond the scope of the present study.