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1 TITLE:

Investigating the Relationship between Sea Surface Chlorophyll and Major Features of the

South China Sea with Satellite Information

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25 satellite observations

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SUMMARY:

Sea surface chlorophyll, temperature, sea level height, wind, and front data obtained or derived from satellite observations offer an effective way to characterize the ocean. Presented is a method for the comprehensive study of these data, including overall average, seasonal cycle, and intercorrelation analyses, to fully understand regional dynamics and the ecosystem.

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ABSTRACT:

Satellite observations offer a great approach to investigate the features of major marine parameters, including include sea surface chlorophyll (CHL), sea surface temperature (SST), sea surface height (SSH), and the factors derived from these parameters (e.g., fronts) which are calculated from the SST gradient. This study shows a step-by-step procedure to use satellite observations to describe major parameters and their relationships in seasonal and anomalous fields. This method is illustrated using satellite datasets from 2002-2017 that were used to describe the surface features of the South China Sea (SCS). Due to cloud coverage, monthly averaged data are used in this study. The empirical orthogonal function (EOF) was applied to describe the spatial distribution and temporal variabilities in different factors. The monsoon wind dominates the variability in the basin. Thus, wind from the reanalysis dataset was used to investigate its driving force on different parameters. The seasonal variability in CHL was

prominent and significantly correlated with other factors in a majority of the SCS. In winter, a strong northeast monsoon induced a deep mixed layer and high level of chlorophyll throughout the basin. Significant correlation coefficients were found among factors during the seasonal cycle. In summer, high CHL levels were mostly found in the western SCS. Instead of seasonal dependence, the region was highly dynamic, and factors correlated significantly in anomalous fields so that unusually high CHL levels were associated with abnormally strong wind and intense frontal activities. The study shows a step-by-step procedure to use satellite observations to describe major parameters and their relationships in seasonal and anomalous fields. The method can be applied to other global oceans and will be helpful for understanding marine dynamics.

INTRODUCTION:

 Remote sensing technology offers great datasets with large spatial scales and long periods for describing marine environments. With the increasing spatial resolution of satellites, detailed features are now resolved from the regional scale to a few hundred meters^{1,2}. An improved understanding of marine dynamics can be achieved with most updated satellite observations³.

By incorporating multiple sensors on a remote sensing platform, a comprehensive description of different parameters is available. Sea surface temperature (SST) is the basic parameter that has been observed for more than half a century⁴. Recently, observations for sea surface chlorophylla (CHL) have become available and can be used to describe marine productivity⁵. Altimetry satellites are used for measuring sea surface height^{6,7}, which is strongly related to mesoscale eddy activities in the global ocean^{8,9}. In addition to eddies, frontal activities are also important for impacting regional dynamics and primary production¹⁰.

The major focus of the current study is to find a standard procedure to describe the spatial distribution and temporal variabilities of different ocean factors. In this method, the SST, CHL, SSH, and front datasets, which are derived from SST, are analyzed to determine patterns. In particular, the CHL is used to represent the productivity of the ocean, and a method is introduced to investigate the relationship between CHL and other ocean parameters. To validate the method, the time period between October 2002 and September 2017 in the South China Sea was used to examine all parameters. The method can be easily used for other regions around the globe to capture major ocean patterns and explore how marine dynamics impact the ecosystem.

The South China Sea (SCS) was designated as the study region because of its relatively high coverage rate of satellite observations. The SCS is abundant in solar radiation; thus, the CHL is mainly determined by the availability of nutrients^{11,12}. With more nutrients being transported into the euphotic layer, CHL levels can increase¹³. Mixing, induced by wind, can introduce nutrients into the ocean surface and enhance CHL¹⁴. The SCS is uniquely dominated by a monsoon wind system, which determines the dynamics and ecosystem in the region. The monsoon wind is strongest during winter¹⁵. In summer, the winds change direction and the wind speeds are much weaker than those in winter^{16,17}. The wind intensity can determine the strength of vertical mixing, such that the mixed layer depth (MLD) deepens as the wind increases in winter and becomes shallower as the wind decreases in summer¹⁸. Thus, more nutrients are transported into the euphotic layer during winter when the wind is strong¹⁹ and CHL reaches its highest point of the

year^{20,21}.

 In addition to the wind, MLD can also be determined using other factors, such as SST and sea level anomaly (SLA), which ultimately impact nutrient content and CHL²². During winter, the weak vertical gradient is associated with low temperatures at the surface²⁰. The corresponding MLD is deep and more nutrients can be transported upward; thus, the CHL in the surface layer is high¹⁷. An increasing variation in CHL levels can be attributed to mesoscale eddies, which induce vertical transport and mixing²³. Upwelling is usually found in cyclonic eddies associated with depressed SLA^{8,9} and elevated CHL²⁴. Downwelling is usually found in anticyclonic eddies associated with elevated SLA^{8,9} and depressed CHL²⁴. For other seasons, MLD becomes shallow, and mixing becomes weak; thus, low CHL can be observed over the majority of the basin²⁵. The seasonal cycles of CHL levels are subsequently predominant for the region²⁶.

In addition to mixing, fronts and their associated coastal upwelling can further modulate the CHL. The front, which is defined as a boundary of different water masses, is important to determine the regional circulation and ecosystem responses²⁷. Frontogenesis is usually associated with coastal upwelling and convergence^{28,29}, which can induce nutrients and elevate the growth of phytoplankton³⁰. Different algorithms have been developed to automatically identify fronts from satellite observations, including histogram and SST gradient methods. The latter approach is adopted in this study²⁸.

The correlation of time series between CHL and different factors offers great insights for quantifying their relationship. The current study offers a comprehensive description of how to use satellite observations to reveal regional marine dynamics related to productivity. This description can be used as a guide for investigating the surface processes in any part of the ocean. The structure of this article includes a step-by-step protocol, followed by descriptive results in the text and figures. The applicability in addition to the pros and cons of the method are subsequently discussed.

PROTOCOL:

1. Dataset acquisition

1.1. SST and CHL

1.1.1. Download a dataset of satellite observations for SST and CHL from MODIS-Aqua (podaactools.jpl.nasa.gov/), where the spatial resolution of both datasets is roughly 4.5 km at daily intervals.

NOTE: Structure the directory of folders and data following the example scripts folder available in the **Supplemental Files**. Store the .nc files of the satellite data in the 'Data' folder. Add the path of the toolbox for NetCDF file in the analysis software (i.e., MATLAB). Select **Add with subfolders** to enclose the paths of the 'UTILITIES' folder and its subfolders.

1.1.2. Determine the time span. To maintain consistency among different datasets, use the same time span for all parameters. Adjust the time span based on the temporal coverage and use the longest observation period among different datasets. For this protocol, download 15 years of data from October 2002 to September 2017.

1.1.3. Determine the spatial coverage.

NOTE: The designed study region is between 105°E and 123°E and between 0° and 25°N.

1.1.4. Check preprocessing instructions. Read instructions in the .nc files regarding the preprocessing requirements of SST and CHL data (e.g., whether scaling is needed).

NOTE: The downloaded dataset already removed the data over land and within 5 km of the coastline, as well as those contaminated by clouds.

1.1.5. Load SST and CHL data into the analysis software. Type **Read_MODIS_SST** in the command window to read the data for SST. Similarly, type **Read_MODIS_CHL** in the command window to read the data for CHL. Transform the CHL data logarithmically because they have a log-normal distribution³¹.

NOTE: Loaded variables include SST and CHL in three dimensions, representing meridional location, zonal location, and time in days, respectively. The range of SSTs is between -2 and 44, and the range of CHL is between 0.01 and 20.

1.2. Sea level anomaly (SLA)

1.2.1. Download daily SLA data with a 25 km spatial resolution from 2002–2017³².

NOTE: SLA describes the difference between the observed sea surface height and the mean sea surface height over 20 years (1993–2012) for the corresponding pixels. The SLA data are processed by SSALTO/DUACS and distributed by Archiving, Validation, and Interpretation of Satellite Oceanographic Data (AVISO, https://www.aviso.altimetry.fr).

1.2.2. Load data into the analysis software. Load single-day SLA data by typing **Read_SLA** in the command window.

NOTE: The 'Data' folder in the **Supplemental Files** only includes one sample datum in the script for illustration.

1.3. Wind speed

1.3.1. Obtain the wind information from an ERA-Interim reanalysis product, which is a global atmospheric reanalysis dataset developed by the European Center for Medium-Range Weather Forecasts (ECMWF)³³. Download wind data for the same period (October 2002–September 2017)

177 to maintain consistency with the CHL and SST data. 178 179 NOTE: The wind dataset has a spatial resolution of approximately 25 km and was interpolated 180 from the original dataset with a spatial resolution of approximately 0.7°. 181 182 1.3.2. Load data into the analysis software. Type **Read_WindVector** in the command window to 183 read the one-month wind data. Calculate the monthly mean by averaging the original data, which 184 is at 6 h intervals. 185 186 1.4. Topography 187 188 1.4.1. Download the high-resolution topography data from the National Centers for 189 Environmental Information website (NCEI, https://maps.ngdc.noaa.gov/viewers/wcs-client/). 190 The spatial resolution is ~2 km. Obtain the ETOPO1 data for bedrock in XYZ format for the 191 selected study region. 192 1.4.2. Load data into the analysis software. Type Read_topography in the command window to 193 194 load the topography data into the analysis software. 195 196 2. Data preprocessing 197 198 2.1. Temporal average 199 200 2.1.1. Due to the large cloud coverage in the SST and CHL data, replace the original data with 3-201 day average data. To do this, after running the Read MODIS SST.m and Read MODIS CHL.m 202 scripts (step 1.1.7), type **Temporal average** in command window to run the script. 203 204 2.2. Interpolation into the same grid 205 206 2.2.1. Because the spatial resolution is not consistent for different datasets, interpolate the SST 207 and CHL data into a spatial grid that is the same as the wind and SLA spatial grid before making 208 comparisons. After running the **Temporal average.m** and **Read WindVector.m** scripts, type 209 **Interpolation** grid in the command window to run the script. 210 211 2.3. Wind stress and wind stress curl 212 213 2.3.1. Type Wind stress curl in the command window to calculate the wind stress (WS) and 214 wind stress curl (WSC) using the following equations: 215 $\vec{\tau} = \rho C \vec{u} \cdot |\vec{u}| \ (1)$ 216

 $\nabla \times \vec{\tau} = \frac{\partial \tau_y}{\partial x} - \frac{\partial \tau_x}{\partial y}$ (2)

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where \vec{u} is the wind speed vector; $\vec{\tau}$ is the WS in the same direction as the wind vector; τ_x and τ_y are the WS in the east and north directions, respectively; ρ is the air density (equal to 1.2 kg/m³); and C is the drag coefficient (a value of 0.0015 is used) under neutral stability conditions³4.

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2.4. Monthly averages

2.4.1. Calculate the monthly SST, wind, and SLA time series as 30-day averages in each pixel by typing **Monthly_average** to run the script. Due to the high cloud coverage rate, use a 60-day average as the monthly time series for CHL, including 30 days before to 30 days after the 15th day of the month.

3. SST front detection

3.1. Spatial smoothing

3.1.1. Type **Spatial_smoothing** to run the script to average the three-day SST data in each pixel.

NOTE: A large amount of noise was identified in the SST data. Thus, data was smoothened with a 3 x 3 spatial average. When no data were available in the original 3-day averaged data, the spatial averaged data were set as unavailable.

3.2. SST gradient

3.2.1. Type **SST_gradient** to run the script to calculate the zonal and meridional SST gradients (i.e., G_x and G_y , respectively) as the SST difference between the nearest two pixels divided by the corresponding distance via equation (3). Use the obtained gradient vector to calculate the total gradient, G_y , as a scalar following equation (4).

$$G_x = \frac{\partial SST_x}{\partial x}$$
, $G_y = \frac{\partial SST_y}{\partial y}$ (3)

$$G = (G_x^2 + G_y^2)^{0.5}$$
 (4)

3.3. Local maximum

3.3.1. Identify a front by testing the value of SST gradient: label the pixel as a potential frontal pixel if the value is larger than a designated threshold. Only maintain the local maximum pixel in the same direction perpendicular to the gradient direction if there are connected pixels with values larger than the threshold. Here, define the threshold as 0.035 °C/km following former studies^{10,28}.

NOTE: The corresponding script 'Local_maximum.m' is available in Supplemental Files.

3.4. Monthly frontal probability (FP)

NOTE: The frontal probability (FP) describes the probability of observing a front take place.

3.4.1. Calculate FP for a certain time span (in this case, the monthly interval), by typing **Monthly_FP** to run the script. Divide the occurrence of fronts at each pixel during a time window by the day number that is free of clouds.

4. Spatial and temporal variability

4.1. Seasonal cycle

4.1.1. Calculate the seasonal cycles of different factors as the averages of different seasons. Define the seasons as follows: winter is from December to February, spring is from March to May, summer is from June to August, and fall is from September to November.

NOTE: The seasonal cycle is not shown in this study; the following method (EOF) is used to explain the spatial and temporal variability instead.

4.2. Empirical orthogonal function (EOF)

4.2.1. Remove the temporal average and unavailable pixels. Before conducting the EOF, subtract the overall mean at each pixel and exclude the locations where missing observations exceed 20% because of cloud coverage. Load data by typing load('Monthly_data_for_EOF.mat') in the command window.

4.2.2. Apply an EOF to describe the spatial and temporal variabilities in different parameters.

Type Empirical_orthogonal_function.m to run the script to calculate the magnitude (Mag),
eigenvalues (Eig), and amplitude (Amp) of the EOFs for the dataset (i.e., time series of monthly
averaged SST, wind stress, wind stress curl, CHL, and FP).

NOTE: The function decomposes the monthly time series into different modes, which are composed of spatial and temporal patterns and the variance explained by each mode decreases with increasing mode number.

5. Intercorrelation

5.1. Correlation at the seasonal scale

5.1.1. Calculate the correlations between two factors using their time series at each pixel by typing **Seasonal_correlation** to run the script. Because the seasonal cycle is not removed, check the significance of the correlation for all correlations.

5.2. Correlation of an anomalous field

5.2.1. Calculate the correlations between the monthly anomalies of the CHL and other factors, such as SST, WS, fronts, and SLA. Obtain the monthly anomalies (i.e., the deviation from the mean status) by subtracting the overall average for the corresponding month from the monthly time series. Type **Anomalous correlation** to run the script and obtain the correlations.

6. Displaying information and calculating relationships

6.1. Display satellite information.

6.1.1. Type **Sat_SCS_Fig3457** to run the script to generate a showcase of satellite information, including SST, CHL, and frontal distribution. Set the current folder as 'scripts' where the data 'Sat_SCS_data.mat' are located.

NOTE: **Figure 1**, **Figure 2**, **Figure 3**, and **Figure 4** show SST, CHL, fronts, wind, and topography for the selected date as an example.

6.2. Display EOF result by typing **Sat_SCS_Fig890.m** to run the script.

NOTE: **Figure 5**, **Figure 6**, and **Figure 7** describe the spatial magnitude, monthly average, and time series of first two modes for CHL, SST, and fronts, respectively.

6.3. Calculate the relationship between chlorophyll and other factors at seasonal and anomalous fields by typing Sat_SCS_Fig1112.m to run the script. Obtain the correlation map for seasonal variability (Figure 8) and anomalous field (Figure 9).

REPRESENTATIVE RESULTS:

The spatial and temporal pattern of sea surface CHL in the SCS was described using satellite observations. Satellite information for CHL (Figure 1A) and SST (Figure 1B) can be contaminated by cloud coverage, which resulted in a large portion of data not being available. The reanalyzed data for wind (Figure 1C) and SLA (Figure 1D) was not impacted by daily clouds. The topography (Figure 1E) had a prominent impact on the spatial distribution of CHL. High CHL was mainly distributed along the coast, where the topography is shallow. Wind was also influenced by orography, and the lee side of mountains was characterized by weak wind; thus, a prominent WSC was identified southwest of the SCS. In contrast, the SLA did not depend much on topography, and an unusually high SLA was found in the basin of the SCS.

[Place Figure 1 here]

Because of the severe cloud impact on satellite observations, a lot of data were either not available or spatially inconsistent. An effective and efficient method was applied to fill some data gaps and smooth the field. The data were first replaced with a 3-day average at each pixel, which can effectively fill some gaps, because clouds vary daily (**Figure 2B**). A spatial average was further applied at each pixel so that the data were replaced by the mean of surrounding values (3 x 3

pixels). Thus, the spatial inconsistency was greatly reduced (Figure 2C).

[Place Figure 2 here]

The daily distribution of the SST front was derived from the SST gradient (**Figure 3A**). The thresholds applied here effectively captured the location of the front (**Figure 3B**) and ensured the depiction of the boundaries of entire water masses (**Figure 3C**). The gradient and front were nearly identical because the front was mainly obtained from the gradient.

[Place Figure 3 here]

Due to cloud coverage in the CHL, SST, and front data, the monthly average time series were calculated and applied in this study. A random example is shown in **Figure 4** for the month of April 2015. There was no existing gap for any of the parameters. The general patterns for different parameters were highly consistent regarding their spatial variance. For example, CHL was high near the coast and low in the central basin, while SST was low near the coast and high in the central basin. The monthly average offered comprehensive information to depict regional features. Fronts were mainly distributed along the coast, where the dynamics are complex. A large portion of the basin was free of fronts; thus, the center of the SCS was characterized by a value close to zero (**Figure 4E**).

[Place Figure 4 here]

Most surface features were characterized by prominent seasonal variability, which was clearly observed using EOFs. The EOF is a useful mathematic method that is widely used in atmospheric and marine sciences. The method can delineate spatial patterns and temporal signals from time series over spatial domains²⁸. After spatiotemporal decomposition for sea surface features in SCS, the first two modes are generally needed for describing the spatial and temporal variabilities. The first two EOFs for CHL described 44% and 12% of the total variance, respectively. EOF1 captured a large variance in the northern section of the SCS (**Figure 5A**). The corresponding monthly average of the time series (**Figure 5C**) showed that the CHL was elevated during the winter and depressed during the summer. The region next to the southwest coast was characterized by weak magnitude, and the corresponding variability was mainly captured by EOF2 (**Figure 5B**). CHL values were high in the summer and low in the winter. This was mainly out of phase compared with the northern section. The monthly time series for EOFs showed clear seasonal variability, and EOF2 led EOF1 by approximately 4 months (**Figure 5E**).

[Place Figure 5 here]

The explained variance in the first two EOFs for SST was prominently high, equaling 91% and 5% for EOF1 and EOF2, respectively. It is important to emphasize that the overall average must be removed before conducting EOF; thus, the mean field was excluded. EOF1 dominated the total variance, and its magnitude was largest in the northern SCS and decreased southward (**Figure 6A**). The corresponding monthly average of the time series (**Figure 6C**) showed that the SST was

elevated during summer and depressed during winter. The southern SCS was characterized by a weak magnitude, attributed to persistent high temperatures at low latitudes. The variability in the southern section was mainly captured by EOF2 (**Figure 6B**). The corresponding SST was enhanced between March and June, while low values persistently occurred in the remaining months. Prominent warming occurred in 2010 and 2016, where the SST off the coast southwest of the SCS was much higher than that in the other years (**Figure 6E**). This interannual variability is mainly attributed to El Niño events that reduce the southwest summer monsoon and result in weak upwelling¹². Because seasonal variability is the major focus of the current study, this feature is not discussed further.

405 [Place Figure 6 here]

Because of the noisy nature of the gradient, the derived front explained much less of the variance. Indeed, EOF1 and EOF2 of FP only explained 19% and 9% of the total variance, respectively. EOF1 captured the variances in the north and northeast SCS (Figure 7A). The corresponding monthly average of the time series (Figure 7C) showed that in those regions, more FP occurred during winter and less during summer. The phase off the coast southwest of the SCS was the opposite, although the corresponding variability was much less prominent. EOF2 captured the spring enhancement of FP (Figure 7D) in the western SCS (Figure 7B). The monthly time series of EOF1 and EOF2 were characterized by weak interannual variability.

[Place Figure 7 here]

Different factors were investigated for their relationships with CHL (**Figure 8**). For example, SST described the fundamental features of the ocean that can influence the growth rate of phytoplankton and subsequently impact CHL. For the majority of the SCS, there were high correlations between SST and CHL (**Figure 8A**), and most of the correlations reached more than -0.8. It is important to point out that high correlation does not indicate causation between these two factors. As SST reached its annual maximum in summer, the MLD became shallowest²¹. Nutrients supplied to the euphotic layer were low because vertical mixing was blocked by intensive stratification¹³. As a result, low nutrients limited the growth rate of phytoplankton and resulted in low CHL. In contrast, high CHL occurred in winter when the MLD was deeper, and low SST induced weak stratification³⁵.

[Place Figure 8 here]

Wind-driven mixing can be approximately gauged by WS and was used to describe vertical mixing¹⁸. Large correlation coefficients, with values of approximately 0.8, were identified between the WS and CHL levels north of the SCS (**Figure 8B**), particularly in the regions with the strongest winter wind located on the northern shelf of the SCS. Weak but significant correlations were found to the south. Correlations between WSC and CHL were significant in the majority of the SCS (**Figure 8C**), although they showed opposing trends in the north and south. The positive correlation coefficient between CHL and WSC was to the south, and the negative values were in the north. The correlation in the region between them was not significant. The WS and CHL were

found to be strongly correlated in the corresponding region where the winter WS was largest.

The front can induce CHL variability. A large correlation was found in the northeast and southwest of the SCS (**Figure 8D**). CHL increased as frontal activities became more active³⁶. The SLA showed a significant negative correlation with CHL from the northeast SCS towards the southwest and a positive correlation along the west coast of the SCS (**Figure 8E**). It is interesting to note that the positive correlations were limited in the region with shallow topography.

To the northeast of the SCS, all the correlations were large (**Figure 8**). Thus, the correlations of monthly time series between CHL and other parameters were calculated using the spatial average in a designated box (**Figure 8A**). The results show that most of the factors were intercorrelated with significant correlations (top right section of **Table 1**). Because the seasonal cycle dominated the time series, the correlation was no longer valid after removing the monthly average (bottom left section of **Table 1**).

[Place Table 1 here]

The correlations in the seasonal cycle were not significant for some regions, such as the southwest of the SCS (**Figure 8**). The region was dominated by dynamic processes (e.g., upwelling and wind-induced offshore transport) that determine the variability in CHL¹⁷. A significant correlation between CHL and other factors (e.g., SST, WS, fronts, and WSC) was identified in anomalous fields (**Figure 9**). The anomalies were calculated for the monthly time series by removing the corresponding monthly average. The effective number of degrees of freedom could be increased, but it did not impact the underlying relationships among their time series^{28, 37}.

[Place Figure 9 here]

In anomalous fields, CHL and SST were significantly correlated in the majority of the SCS (Figure 9A). When SSTs were unusually high, CHL became unusually low, and vice versa. Similarly, an unusually high WSC and fronts to the southwest of the SCS can induce a large CHL, and vice versa (Figure 9C, 9D). In addition, a negative correlation was found between the anomalous SLA and CHL levels (Figure 9E). Different lags were tested, and the correlation only became significant if no lag was deployed. Thus, CHL was simultaneously impacted by anomalies in SST, WSC, fronts, and SLA. Their relationship was further investigated using the spatially averaged monthly time series southwest of the SCS, designated as a green box in Figure 9A. The results show that most of the factors were intercorrelated with significant correlations in the anomalous field (bottom left section of Table 2).

[Place Table 2 here]

FIGURE AND TABLE LEGENDS:

Figure 1: Original observations for major parameters on April 15, 2015. (A) Sea surface chlorophyll (CHL), (B) sea surface temperature (SST), (C) wind stress curl (WSC, shading) with wind stress (WS, vector), (D) sea surface anomaly, and (E) topography for the ocean basin.

Figure 2: SST for a single day on April 15, 2015. (A) Original SST from MODIS, (B) Three-day averaged SST, and (C) SST after spatial smoothing.

Figure 3: Procedure for front detection derived from SST. (A) Magnitude of SST gradient, **(B)** the distribution of the SST front in thin black color, and **(C)** front distribution with the corresponding SST.

Figure 4: Monthly average for major parameters in April 2015. (A) CHL (in logarithm scale), (B) SST, (C) WSC (shading) with WS (vector), (D) sea surface anomaly, and (E) frontal probability (FP).

Figure 5: The EOF for CHL. (A) Magnitude of EOF1, **(B)** magnitude of EOF2, **(C)** monthly averaged time series for EOF1, **(D)** monthly average time series for EOF2, and **(E)** monthly time series of EOF1 (black) and EOF2 (blue).

Figure 6: The EOF for SST. (A) Magnitude of EOF1, (B) magnitude of EOF2, (C) monthly averaged time series for EOF1, (D) monthly averaged time series for EOF2, and (E) monthly time series of EOF1 (black) and EOF2 (blue).

Figure 7: The EOF for FP. (A) Magnitude of EOF1, (B) magnitude of EOF2, (C) monthly averaged time series for EOF1, (D) monthly averaged time series for EOF2, and (E) monthly time series of EOF1 (black) and EOF2 (blue).

Figure 8: Correlations between CHL and other factors in the seasonal scale. (A) SST, (B) WS, (C) WSC, (D) FP, and (E) SLA. The gray color indicates that the correlation is nonsignificant. Spatially averaged variables are calculated based on the green box in panel A. Their time series are used to obtain the correlation coefficients in **Table 1**. This figure has been modified from Yu et al.¹⁷.

Figure 9: Correlation between CHL and other factors in the anomalous field. (A) SST, (B) WS, (C) WSC, (D) FP, and (E) SLA. The gray color indicates that the correlation is nonsignificant. Spatially averaged variables are calculated based on the green box in panel A Their time series are used to obtain the correlation coefficients shown in Table 2. This figure has been modified from Yu et al.¹⁷.

Table 1: Correlation coefficients of the time series among factors, located northeast of the SCS, e.g., SST (sea surface temperature), FP (frontal probability), WSC (wind stress curl) and WS (wind stress), using the box shown in Figure 8A. The monthly average and anomaly are shown in the top right section and left bottom section, respectively. Numbers in bold and italics indicate that the correlation cannot fulfill the 95% confidence level. The table has been modified from Yu et al.¹⁷.

Table 2: Correlation coefficients of the time series among factors, located southwest of the SCS, e.g., SST (sea surface temperature), FP (frontal probability), WSC (wind stress curl) and WS (wind stress), using the box shown in Figure 9A. The monthly average and anomaly are shown

in the top right section and left bottom section, respectively. Numbers in bold and italics indicate that the correlation cannot fulfill the 95% confidence level. The table has been modified from Yu et al. 17 .

DISCUSSION:

In this study, the major features of marine systems are described using satellite observations. The CHL, which can be used to represent ocean production, is selected as an indicator factor. Factors related to CHL variability were investigated using monthly averaged time series, e.g., SST, WS, WSC, FP and SLA. Three critical steps are described in this study: acquiring satellite data for different parameters, describing their spatial and temporal variabilities via EOF, and determining interrelationships among different factors by calculating correlation coefficients. A detailed procedure showing the identification for daily frontal distribution, which is derived from the SST observations, is included. Two major approaches have been developed for SST front detection: the gradient method^{10,38} and the histogram method^{39,40}. The histogram method is based on a similar range of values for SST, which can be used to divide the water masses into different groups. The Pixels with values between different groups representing the pixel in a transitional band are defined as fronts. On the other hand, the gradient method separates several relatively uniform water bodies as pixels with large gradient values. A comparison study was conducted, and they found lower false rates using the histogram method and fewer missed fronts using the gradient method⁴¹. In this study, the gradient-based method³⁸ was adopted following former studies 10,28. The algorithm can avoid front break-up into multiple edge fragments by allowing the magnitude to decrease to a level below a smaller threshold. In addition to the dataset included here, other satellite observations, such as the aerosol index, can also be used with a similar approach.

Most of the procedures can be directly applied in other regions or datasets. Modification may take place to change the threshold of front detection. Because the SST gradient in the SCS is comparable with the Eastern Boundary Current System²⁸, the same thresholds were implemented for the current study. A previous study revealed that the SST gradient from different datasets can vary as much as three times⁴², which makes the method somehow less objective. Substantial studies have investigated frontal activities around the global oceans^{28,43}. The best approach to validate fronts is to compare them with in situ observations. Yao⁴⁴ described the monthly frontal distribution for the SCS. Their results agreed well with the in situ measurements. The overall gradient should be checked and adjusted since its value may vary depending on the spatial resolution and instruments. In particular, the threshold should be updated when another SST dataset is used. A basic understanding of the regional dynamics is fundamental to understanding frontogenesis^{45,46,47}. The front detection script can be developed by individual authors based on the description in this paper.

Satellite information offers a comprehensive understanding of surface features, and a results comparison with in situ observations can aid in evaluating credibility. However, satellite observations are limited to the ocean surface, which limits the application for understanding the vertical structure of the water column. In a recent study, satellite observations revealed that the surface CHL increased by 15 times, but the vertical integrated value only increased by 2.5 times⁴⁸.

This difference was because the surface value was impacted by the coeffects of phytoplankton growth and shoaling of MLD, resulting in an unrealizable value at the surface. Thus, the surface feature may not offer an accurate description for the entire water column. Additionally, the influence of cloud coverage limits the continuous observations of satellites. Thus, monthly time series are calculated for different factors over the same region and same period. This will guarantee the credibility of calculating the correlations among different factors. However, the short-period events, e.g., typhoons that last for a few days to a week, will not be resolved.

Compared with former studies, the proposed method can offer spatial information at the pixel level, which can help to evaluate the dynamics in a more detailed manner. Some former studies averaged the entire SCS as a single number and obtained a time series. They found that an unusually strong WS and high SST can induce anomalously high CHL¹⁶, which is consistent with current result. However, the spatial variation in the relationships was not resolved. In this study, the basin-scale correlation between WS and CHL was weak in the anomalous field. A large significant correlation was only identified for certain areas, e.g., in the center of the SCS (**Figure 9B**). Thus, the current method offers a comprehensive description for investigating spatial variations. Similarly, observations from two Bio-Argo floats were used and revealed that WSC did not correlate with CHL variability²⁰. However, the trajectories of the two floats are only located in certain regions. In this case, it was exactly within the band where the correlation between the CHL level and the WSC was not significant (**Figure 8D**). The proposed method is very helpful for resolving the spatial dependence among factors, which is a fundamental characteristic of the global ocean.

In summary, the method used here can accurately describe the spatial distribution and temporal variability in ocean surface features using satellite observations. With the increasing resolution of satellite datasets, more detailed features can be identified and investigated, which enables a general understanding of regional features, including CHL, SST, and SSH. The correlation of monthly time series among different factors can aid in understanding their dynamic relationships and potential impact on an ecosystem⁴⁹. Because the correlation can largely vary at different spatial locations, the proposed method offers a detailed and comprehensive description. A similar approach can be applied to any ocean basin worldwide, which will be greatly helpful to improve the understanding of marine dynamics and ecosystems.

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DISCLOSURES:

The authors have nothing to disclose.

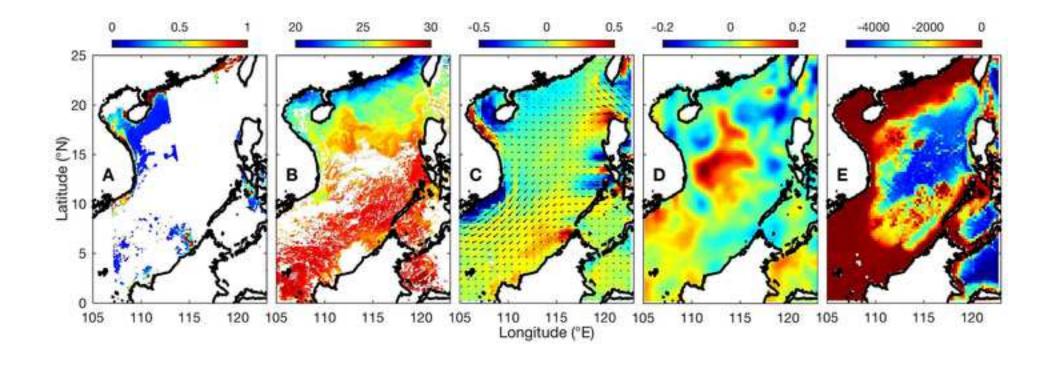
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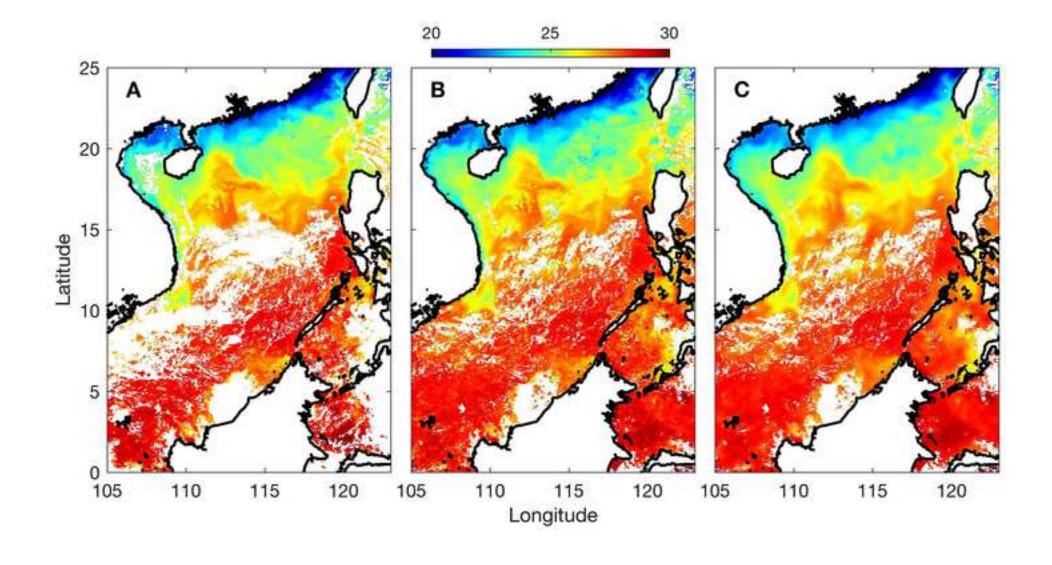
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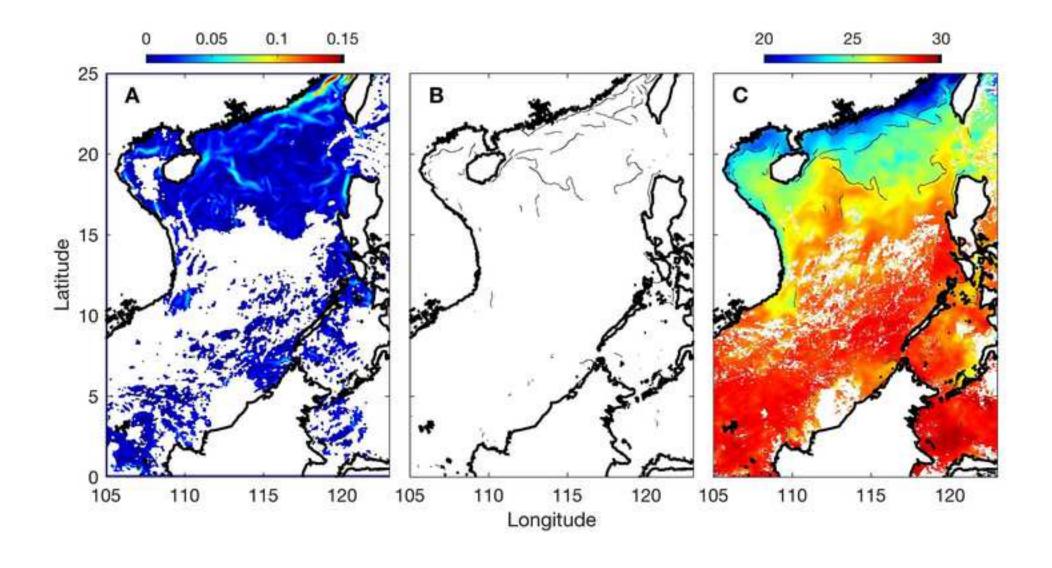
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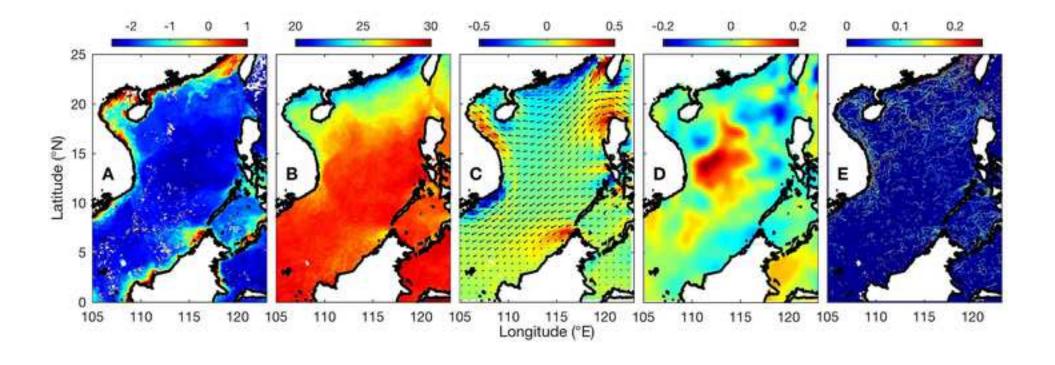
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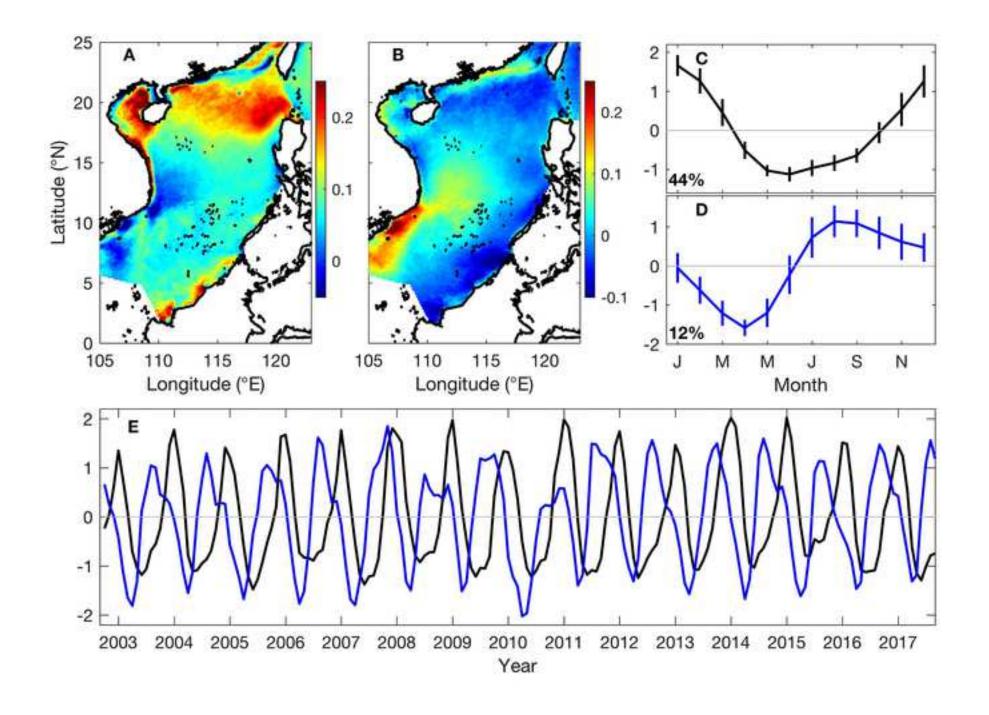
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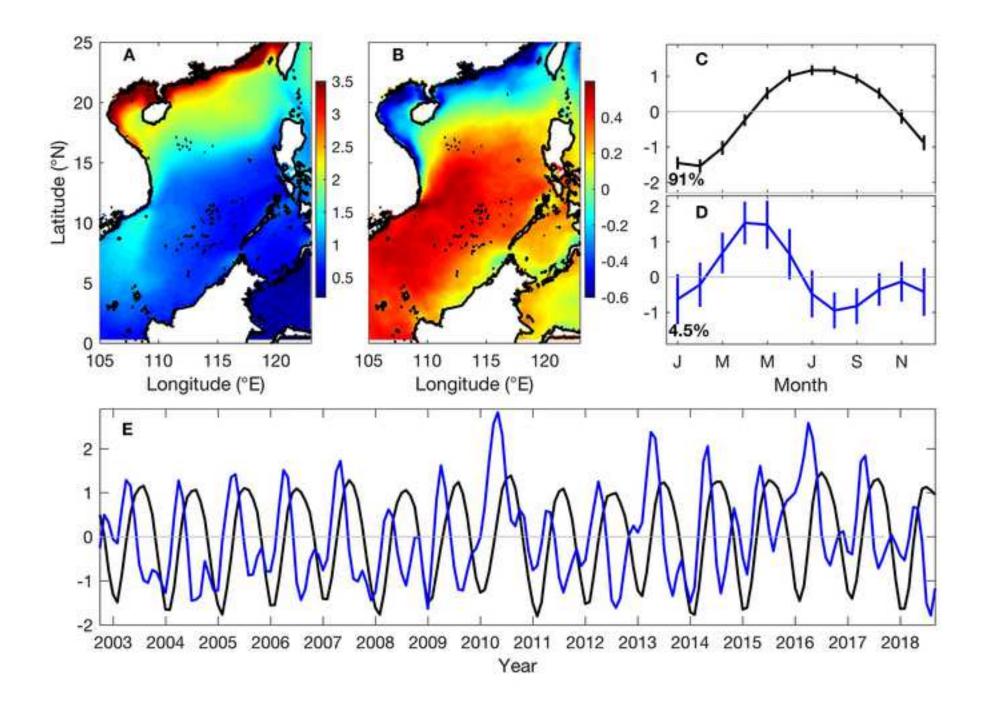


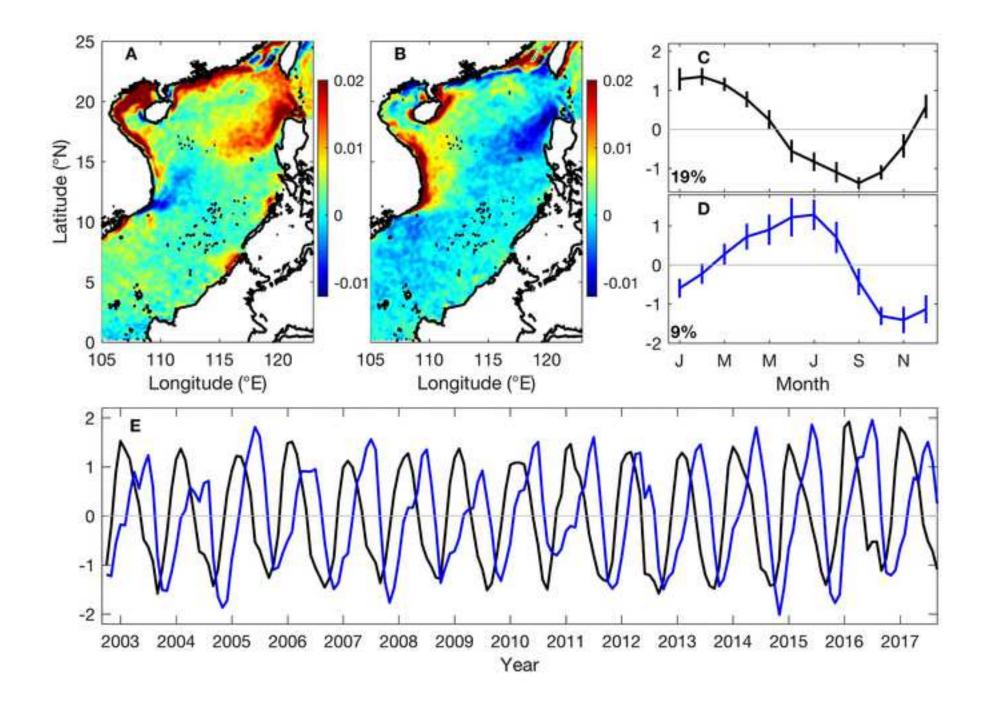


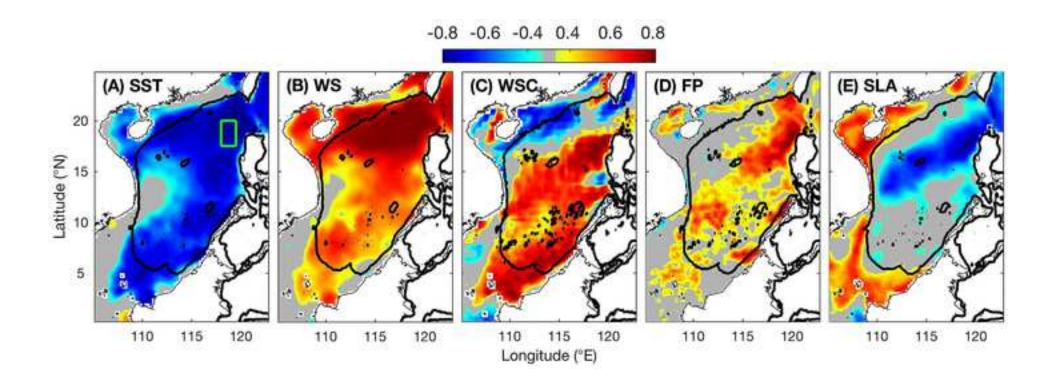


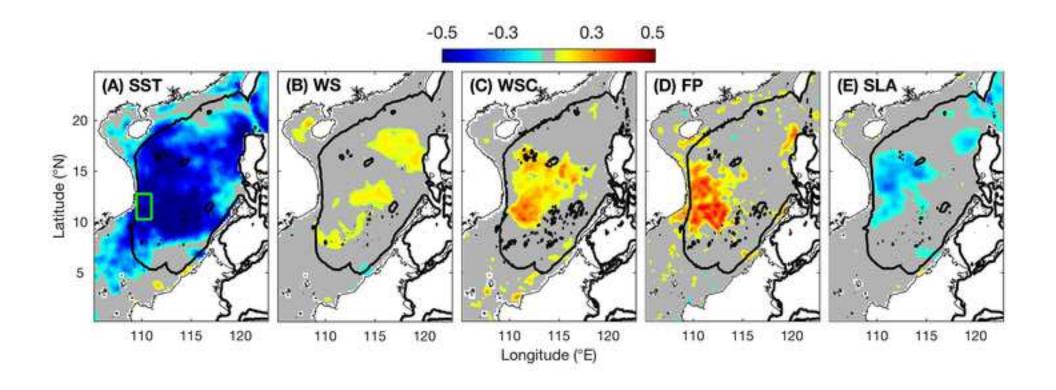












	Chl-a	SST	WS	WSC	FP	SLA
Chl-a		-0.8	0.78	0.67	0.74	-0.71
SST	-0.41		-0.47	-0.51	-0.79	0.86
WS	0.32	0.04		0.63	0.51	-0.38
WSC	0	0.08	-0.02		0.52	-0.37
FP	0.21	-0.09	0.03	0.15		-0.74
SLA	-0.25	0.42	0.07	0.13	-0.08	

	Chl-a	SST	WS	WSC	FP	SLA
Chl-a		-0.15	0.36	0.35	0.26	-0.15
SST	-0.59		-0.48	0.61	0.07	0.17
WS	0.25	-0.24		-0.14	-0.02	0.1
WSC	0.29	-0.1	0.41		0.53	-0.21
FP	0.57	-0.42	0.24	0.29		-0.42
SLA	-0.3	0.54	-0.23	-0.29	-0.47	

Name of Material/Software	Agent/Company	Dateset/Catalog N Comments/Description		
Matlab	MathWorks	Matlab R2016	https://www.mathworks.com/products/matlab.html; referred to analysis soft	
Sea surface chlorophyll	NASA	MODIS	mg/mg ³ (podaac-tools.jpl.nasa.gov)	
Sea surface height	AVISO	AVISO	meter (www.aviso.altimetry.fr)	
Sea surface temperature	NASA	MODIS	°C (podaac-tools.jpl.nasa.gov)	
Topography	NOAA	NGDC	meter (maps.ngdc.noaa.gov/viewers/wcs-client/)	
Wind	ECMWF	ERA-interim	m/s (www.ecmwf.int/en/forecasts/datasets)	

tware in the protocol

TITLE:

Using Satellite Information to Investigate Sea Surface Chlorophyll and its Relationship with Major Features in the South China Sea

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KEYWORDS:

chlorophyll, sea surface temperature, sea surface height, South China Sea, seasonal cycle, satellite observations

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SUMMARY:

The sea surface chlorophyll, temperature, sea level height, wind and front data obtained or derived from satellite observations offer an effective way to characterize the ocean. A comprehensive analysis of these data is conducted, including overall average, seasonal cycle, and intercorrelation analyses, to fully understand its regional dynamics and ecosystem.

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ABSTRACT:

Satellite observations offer a great approach to investigate the features of major marine parameters. In this study, satellite datasets from 2002 to 2017 were used to describe the surface features in the South China Sea (SCS). Major parameters include sea surface chlorophyll (CHL); sea surface temperature (SST); sea surface height (SSH); and factors derived from these parameters, e.g., fronts, which were calculated from the SST gradient. Due to cloud coverage, monthly averaged data are used in this study. The empirical orthogonal function (EOF) is applied to describe the spatial distribution and temporal variabilities in different factors. The monsoon wind dominates the majority of the variability in the basin; thus, wind from the reanalysis dataset is used to investigate its driving force on different parameters. The seasonal variability in CHL was indeed prominent and significantly correlated with other factors in a majority of the SCS. In winter, a strong northeast monsoon induces a deep mixed layer and high level of chlorophyll throughout the basin. Significant correlation coefficients are found among factors during the seasonal cycle. In summer, high CHL levels were mostly found in the western SCS. Instead of seasonal dependence, the region is highly dynamic, and factors are significantly correlated in anomalous fields such that anomalously high CHL levels are associated with abnormally strong wind and intense frontal activities. The study showed a step-by-step procedure regarding how to use satellite observations to describe major parameters and their relationships in seasonal and anomalous fields. The method can be applied in other global oceans and will be helpful for understanding marine dynamics.

INTRODUCTION:

The development of remote sensing technology offers a great dataset for describing marine environments with large spatial scales and long periods. With the increasing spatial resolution of satellites, detailed features are now resolved from the regional scale to a few hundred meters^{1,2}. An improved understanding of marine dynamics can be achieved with most updated satellite observations³.

By incorporating multiple sensors on the remote sensing platform, a comprehensive description is available for different parameters. Sea surface temperature (SST) is the basic parameter that has been observed for more than half century⁴. Recently, observations for sea surface chlorophyll-a (CHL) have become available and can be used to describe marine productivity⁵. Altimetry satellites are used for measuring sea surface height^{6,7}, which is highly related to mesoscale eddy activities in the global ocean^{8,9}. In addition to eddies, frontal activities are also important for impacting regional dynamics and primary production¹⁰. In this study, the SST, CHL, SSH and front datasets, which are derived from SST, are used to analyze their patterns. The time period between October 2002 and September 2017 is used for all parameters.

A major focus of the current study is to find a standard procedure to describe the spatial distribution and temporal variabilities in different factors. In particular, the CHL is used to represent the productivity of the ocean, and a method can be widely used is introduced to investigate the relationship between CHL and other ocean parameters. The method can be used in the future for other regions around the globe to capture major ocean patterns and explore how marine dynamics impact the ecosystem.

The South China Sea (SCS) is designated as the study region because of its relatively high coverage rate of satellite observations. The SCS is abundant in solar radiation; thus, the CHL is mainly determined by the availability of nutrients ^{11,12}. With more nutrients being transported into the euphotic layer, the CHL levels can increase ¹³. Mixing, induced by wind, can introduce nutrients into the ocean surface and enhance CHL¹⁴. The SCS is uniquely dominated by a monsoon wind system, which subsequently determines the dynamics and ecosystem in the region. The monsoon wind is strongest during winters each year ¹⁵. In summer, the winds change direction and the wind speeds are much weaker than those in winter ^{16,17}. The wind intensity can determine the strength of vertical mixing such that the mixed layer depth (MLD) deepens (shoal) as the wind increases (decreases) ¹⁸. More nutrients will be transported into the euphotic layer during winter when the wind is strong ¹⁹ and CHL reaches its highest point over the year ^{20,21}.

In addition to the wind, MLD can also be determined by other factors, e.g., SST and sea level anomaly (SLA), which ultimately impact nutrient content and CHL²². During winter, the weak vertical gradient is associated with low temperatures at the surface²⁰. The corresponding MLD is deep, and more nutrients can be transported upward; thus, the CHL in the surface layer is high¹⁷. An increasing variation in CHL levels can be attributed to mesoscale eddies, which induce vertical transport and mixing²³. Upwelling (downwelling) is usually found in cyclonic (anticyclonic) eddies associated with depressed (elevated) SLA^{8,9} and elevated (depressed) CHL²⁴. For other seasons, MLD becomes shallow, and mixing becomes weak; thus, low CHL can be observed over the majority of the basin²⁵. The seasonal cycles of CHL levels are subsequently predominant for the region²⁶.

In addition to mixing, fronts and their associated coastal upwelling can further modulate the CHL. The front, which is defined as a boundary of different water masses, is important to determine the regional circulation and ecosystem responses²⁷. Frontogenesis is usually associated with coastal upwelling and convergence^{28,29}, which can induce nutrients and elevate the growth of phytoplankton³⁰. Different algorithms have been developed to automatically identify fronts from satellite observations, including histogram and SST gradient methods, and the latter approach is adopted in this study²⁸.

The correlation of time series between CHL and different factors offers great insights for quantifying their relationship. The current study offers a comprehensive description of how to use satellite observations to reveal regional marine dynamics related to productivity. This description can be used as a guide for investigating the surface processes in any part of the ocean. The structure of the manuscript includes a step-by-step protocol in the next section, followed by descriptive results in the text and figures. The applicable situation and pros/cons of the method are subsequently discussed.

PROTOCOL:

1. Dataset acquisition

1.1. SST and CHL

1.1.1. Download dataset. Obtain a dataset of satellite observations for SST and CHL from MODISAqua (podaac-tools.jpl.nasa.gov/) where the spatial resolutions of both of these data are approximately 4.5 km at daily intervals (Figure S1).

[Place Figure 1 here]

1.1.2. Determine time span. To maintain consistency among different datasets, use the same time span for all parameters. Adjust the time span based on their temporal coverage and use the longest observing period among different datasets. In this study, download 15 years of data from October 2002 to September 2017.

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1.1.3. Perform spatial configuration. Remove the data over land and within 5 km of the coastline, as well as those contaminated by clouds. Transform the CHL data logarithmically because they have a log-normal distribution³¹.

NOTE: The designed study region is between 105°E and 123°E and between 0° and 25°N. Downloaded dataset already removed the data over land and within 5 km of the coastline, as well as those contaminated by clouds.

1.1.4. Check preprocessing instruction. Read instructions in the .nc files regarding the preprocessing of SST and CHL data, e.g., scaling is not needed for the SST and CHL data.

NOTE: The range of SSTs is between -2 and 44, and the range of CHL is between 0.01 and 20.

1.1.5. Add the path of the toolbox for NetCDF file in Matlab (Figure 2). Use the option 'Add with subfolers' to enclose the paths of the folder 'UTILITIES' and its subfolders (Figure S2).

NOTE: All required functions are enclosed in the supplementary folder.

[Place Figure 2 here]

1.1.6. Load and store data into Matlab. Type 'Read MODIS SST.m' in the command window to Read-read the data for SST. Similarly, type 'Read MODIS CHL.m' in the command window to read the data for and CHL by running 'Read MODIS SST.m' and 'Read MODIS CHL.m', respectively, via clicking the 'RUN' button (Figure S3). Store the .nc files of the satellite data in the folder 'Data'. Structure directory of folders and data following supplementary file.

NOTE: The output variables include SST and CHL in three dimensions, representing meridional location, zonal location and time in days, respectively.

[Place Figure 3 here]

1.2. Sea level anomaly (SLA)

1.2.1. Download daily SLA data with a 25 km spatial resolution from 2002 to 2017³². The SLA data are processed by SSALTO/DUACS and distributed by Archiving, Validation and Interpretation of Satellite Oceanographic Data (AVISO, https://www.aviso.altimetry.fr).

NOTE: SLA describes the difference between the observed sea surface height and the mean sea surface height over 20 years (1993-2012) for the corresponding pixels. The SLA data are processed by SSALTO/DUACS and distributed by Archiving, Validation and Interpretation of Satellite Oceanographic Data (AVISO, https://www.aviso.altimetry.fr).

1.2.2. Load and read single-day SLA data by typing 'Read SLA.m' in the command window and

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177 clicking Run (Figure \$4).

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NOTE: Supplementary folder only includes one sample datum in the script for illustration.

[Place Figure 4 here]

1.3. Wind speed

1.3.1. Obtain the wind information from an ERA-Interim reanalysis product, which was a global atmospheric reanalysis dataset developed by the European Center for Medium-Range Weather Forecasts (ECMWF)³³. The dataset has a spatial resolution of approximately 25 km and was interpolated from the original dataset with a spatial resolution of approximately 0.7°. Download data for the same period (between October 2002 and September 2017) to maintain consistency with the CHL and SST data.

1.3.2. Load data into Matlab. Type 'Read_WindVector' in the command window and click Run-to read the one-month wind data (Figure S5). Calculate the monthly mean by averaging the original data, which is at 6-h intervals.

[Place Figure 5 here]

1.4. Topography

1.4.1. Download the high-resolution topography data from the website of the National Centers for Environmental Information (NCEI, https://maps.ngdc.noaa.gov/viewers/wcs-client/)-(Figure 6). The spatial resolution is approximately 2 km. Obtain the ETOPO1 data for bedrock in xyz format for the selected study region (Figure S6).

[Place Figure 6 here]

1.4.2. Load data into Matlab. Obtain the ETOPO1 data for bedrock in xyz format for the selected study region. Type 'Read_topography.m' in the command window and click Run to read the topography (Figure \underline{S} 7).

[Place Figure 7 here]

2. Data preprocessing

2.1. Temporal average

2.1.1. Due to the large cloud coverage in the SST and CHL data, replace the original data with 3-day average data. To do this, after running the 'Read_MODIS_SST.m' and 'Read_MODIS_CHL.m' scripts (step 1.1.6), type 'Temporal_average.m' in the command window to and click Rrun the script -(Figure S8).

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NOTE: The data are handled at each pixel for each time step. (Note that the script is run)

[Place Figure 8 here]

2.2. Interpolation into the same grid

2.2.1. Because the spatial resolution is not consistent for different datasets, interpolate the SST and CHL data into a spatial grid that is the same as the wind and SLA spatial grid before making comparisons. Use the script 'Interpolation_grid.m' after After running the 'Temporal_average.m' and 'Read_ WindVector.m' scripts, type 'Interpolation_grid.m' in the command window to run the script (Figure S9).

234 [Place Figure 9 here]

2.3. Wind stress (curl)

2.3.1. Run the script "Wind_stress_curl.m" (Figure §10) to calculate the wind stress (WS) and wind stress curl (WSC) using the following equations:

$$\vec{\tau} = \rho C \vec{u} \cdot |\vec{u}| (1)$$

$$\nabla \times \vec{\tau} = \frac{\partial \tau_y}{\partial x} - \frac{\partial \tau_x}{\partial y} (2)$$

where \vec{u} is the wind speed vector; $\vec{\tau}$ is the WS in the same direction as the wind vector; τ_x and τ_y are the WS in the east and north directions, respectively; ρ is the air density (equal to 1.2 kg/m³); and C is the drag coefficient (a value of 0.0015 is used) under neutral stability conditions³4.

[Place Figure 10 here]

2.4. Monthly average

2.4.1. Calculate the monthly SST, wind and SLA time series as 30-day averages in each pixel by running 'Monthly_average.m' (Figure §11). Due to the high cloud coverage rate, use a 60-day average as the monthly time series for CHL, including 30 days before to 30 days after the 15th day of the month.

[Place Figure 11 here]

3. SST front detection3.1. Spatial smoothing

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3.1.1. Use-Run the 'Spatial_smoothing.m' script to average the three-day SST data in each pixel (Figure S12).

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[Place Figure 12 here]

3.2. SST gradient

3.2.1. Run 'SST_gradient.m' to calculate the zonal and meridional SST gradients (G_X and G_Y , respectively) as the SST difference between the nearest two pixels divided by the corresponding distance via (Figure $\underline{S}13$) following equations (3). Use the obtained gradient vector to calculate the total gradient, G_X , as a scalar following equation (4).

NOTE: Large noise was identified in the SST data; thus, smooth data with a 3*3 spatial average

were used. When no data were available in the 3-day averaged data, these data were set as

$$G_x = \frac{\partial SST_x}{\partial x}, G_y = \frac{\partial SST_y}{\partial y} (3)$$
$$G = (G_x^2 + G_y^2)^{0.5} (4)$$

[Place Figure 13 here]

3.3. Local maximum

3.3.1. Identify a front by testing the value of SST gradient, e.g., label the pixel as a potential frontal pixel if the value is larger than a designated threshold. Only maintain the local maximum pixel in the same direction perpendicular with the gradient direction if there are connected pixels with values larger than the threshold (Figure $\underline{S}14$). Here, define the threshold equal to 0.035 °C/km following former studies $\underline{S}10.28$.

NOTE: Find corresponding scripts in the supplementary document as 'Local maximum.m'.

[Place Figure 14 here]

3.4. Monthly frontal probability (FP)

NOTE: The frontal probability (FP) describes the probability when the front takes place.

3.4.1. Calculate FP for a certain time span, which in this case is the monthly interval by running 'Monthly FP.m' (Figure S15). Divide the occurrence of fronts at each pixel during a time window by the day number that is free of clouds.

[Place Figure 15 here]

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4. Spatial and temporal variability

4.1. Seasonal cycle

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4.1.1. Calculate the seasonal cycles of different factors as the averages of different seasons, Here, define the seasons as follows: winter is from Dec. to Feb., spring is from March to May, summer is from Jun. to Aug., and fall is from Sep. to Nov.

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4.1.1. NOTE: The seasonal cycle is not shown in this study, the following method (EOF) is used to explain the spatial and temporal variability instead.

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4.2. Empirical orthogonal function (EOF)

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4.2.1. Remove temporal average and unavailable pixels. <u>Load data by typing</u> <u>'load('Monthly data for EOF.mat')' in the command window.</u> Apply an empirical orthogonal function (EOF) to describe the spatial and temporal variabilities in different parameters. Before conducting the EOF, subtract the overall mean at each pixel and exclude the locations where missing observations exceed 20% because of cloud coverage.

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1.1.1.

NOTE: The function decomposes the monthly time series into different modes, which are composed of spatial and temporal patterns and the variance explained by each mode decreases with increasing mode number.

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4.2.1. Load data by typing 'load('Monthly_data_for_EOF.mat')' in the command window.

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4.2.2. Apply an empirical orthogonal function (EOF) to describe the spatial and temporal variabilities in different parameters. Run the script 'Empirical_orthogonal_function.m' to calculate the magnitude (Mag), eigenvalues (Eig) and amplitude (Amp) of the EOFs for dataset (i.e., time series of monthly averaged SST, wind stress, wind stress curl, CHL and FP; Figure S16).

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NOTE: The function decomposes the monthly time series into different modes, which are composed of spatial and temporal patterns and the variance explained by each mode decreases with increasing mode number.

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[Place Figure 16 here]

5. Intercorrelation

5.1. Correlation at the seasonal scale

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5.1.1. Calculate the correlations between two factors using their time series at each pixel via 'Seasonal_correlation.m' (Figure $\underline{S}17$). Because the seasonal cycle is not removed, check the significance of the correlation for all correlations.

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B51 [Place Figure 17 here]

5.2. Correlation of an anomalous field

5.2.1. Calculate the correlations between the monthly anomalies of the CHL and other factors, such as SST, WS, fronts and SLA. Obtain the monthly anomalies (the deviation from the mean status) by subtracting the overall average for the corresponding month from the monthly time series. Use the script 'Anomalous correlation.m' to obtain the correlations (Figure §18).

[Place Figure 18 here]

6. Display information and calculate relationship REPRESENTATIVE RESULTS:

6.1. 6.1 Display satellite information

6.1.1

Satellite observations for CHL and SST can be contaminated by cloud coverage, which results in a large portion of data that is not available. Run 'Sat_SCS_Fig3457.m' (Figure 19) is run to produce Figures 221 to Figure, 23, 24 and 284 about satellite information. The Set current folder is ensured to be set toas 'scripts' where the data 'Sat_SCS_data.mat' are located (Figure S19).

6.2. 6.2 Display EOF result

6.2.1 Run 'Sat SCS Fig890.m' to produce Figure 5 to Figure 7 about display EOF results (Figure S20). Figure 5 to Figure 7 describe the spatial magnitude, monthly average and time series of first two modes for CHL, SST and fronts, respectively.

6.3. 6.3-Calculate relationship between chlorophyll and others

<u>6.3.1 Run 'Sat SCS Fig1112.m' to calculate the relationship between chlorophyll and other factors at seasonal and anomalous field (Figure S21). Obtain the correlation map shown as Figure 8 and Figure 9.</u>

REPRESENTATIVE RESULTS:

[Place Figure 19 here]

Satellite observations for CHL (Figure 1A) and SST (Figure 1B) can be contaminated by cloud coverage, which results in a large portion of data that is not available. The reanalyzed data for wind (Figure 1C) and SLA (Figure 1D) areis not impacted by daily clouds. The topography (Figure 1E) has a prominent impact on the spatial distribution of CHL (Figure 20). High CHL is mainly distributed along the coast where the topography is shallow (Figure 20E). Wind is also influenced by orography, and the lee side of mountains is characterized by weak wind; thus, a prominent WSC can be identified, e.g., southwest of the SCS. In contrast, the SLA does not depend much on

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[Place Figure 20-1 here]

Because of the severe cloud impact on satellite observations, many data are not available or spatially inconsistent. An effective and efficient method is applied to fill some data gaps and smooth the field. The data are first replaced with a 3-day average at each pixel, which can effectively fill some gaps as the cloud varies on a daily basis (Figure 21B). A spatial average is further applied at each pixel such that the data are replaced by the mean of surrounding values (3*3 pixels). Thus, the spatial inconsistency can be greatly reduced (Figure 21C). The locations where satellite data are unavailable after a 3-day average remain unavailable (the blank regions are the same for Figure 21B and Figure 21C).

[Place Figure 24 here]

The daily distribution of the SST front is derived from the SST gradient (Figure 322A). The thresholds applied here can effectively capture the location of the front (Figure 322B) and ensure depiction of the boundaries of entire water masses (Figure 322C). In comparing the gradient and front, they are highly identical because the front is mainly obtained from the gradient.

[Place Figure 322 here]

Due to cloud coverage in the CHL, SST and front data, the monthly average time series are calculated and applied in this study. A random example is shown in Figure 23.4 for the month of April 2015. There is no existing gap for any of the parameters. The general patterns for different parameters are highly consistent regarding their spatial variance. For example, CHL (SST) is high (low) near the coast and low (high) in the central basin. The monthly average can offer comprehensive information for depicting the regional features. Fronts are mainly distributed along the coast where the dynamics are complex. A large portion of the basin is free of fronts; thus, the center of the SCS is characterized by a value close to zero (Figure 423E).

[Place Figure 23-4 here]

Most of the surface features are characterized by prominent seasonal variability, which can be clearly observed by EOFs (Figure 24). EOF is a useful mathematic method, which has been widely used in atmospheric and marine sciences. The method can delineate spatial patterns and temporal signals from time series over spatial domains²⁸. After spatiotemporal decomposition for sea surface feature in SCS, the first two modes are generally needed for describing the spatial and temporal variabilities. The first two EOFs for CHL describe 44% and 12% of the total variance, respectively. EOF1 captured a large variance in the northern section of the SCS (Figure 25A). The corresponding monthly average of the time series (Figure 25C) shows that the CHL is elevated (depressed) during winter (summer). The region next to the southwest coast is characterized by a weak magnitude, and the corresponding variability is mainly captured by EOF2 (Figure 25B). High (low) CHL values occur during summer (winter), which is mainly out of phase compared with

the northern section. The monthly time series for EOFs show clear seasonal variability, and EOF2 leads EOF1 by approximately 4 months (Figure 25E).

[Place Figure 24 here]

[Place Figure 25 here]

The explained variance in the first two EOFs for SST is prominently high, equaling 91% and 5% for EOF1 and EOF2, respectively. It is important to emphasize that the overall average be removed before conducting EOF; thus, the mean field is excluded. EOF1 dominates the total variance, and its magnitude is largest in the northern SCS and decreases southward (Figure 26A). The corresponding monthly average of the time series (Figure 26C) shows that the SST is elevated (depressed) during summer (winter). The southern SCS is characterized by a weak magnitude, which is attributed to persistent high temperatures at low latitudes. The variability in the southern section is mainly captured by EOF2 (Figure 26B). The corresponding SST is enhanced between March and June, while low values persistently occur in the remaining months. Prominent warming occurred in 2010 and 2016, where the SST off the coast southwest of the SCS was much higher than that in the other years (Figure 26E). This interannual variability is mainly attributed to El Niño events that reduce the southwest summer monsoon and result in weak upwelling¹². Because seasonal variability is the major focus of the current study, this feature will not be further discussed.

[Place Figure 26 here]

Because of the noisy nature of the gradient, the derived front explained much less of the variance. Indeed, EOF1 and EOF2 of FP only explained 19% and 9% of the total variance, respectively. EOF1 captured the variances in the north and northeast SCS (Figure 27A). The corresponding monthly average of the time series (Figure 27C) shows that more (less) FP occurs during winter (summer) in those regions. The phase off the coast southwest of the SCS is the opposite, although the corresponding variability is much less prominent. EOF2 captures the spring enhancement of FP (Figure 27D) in the western SCS (Figure 27B). The monthly time series of EOF1 and EOF2 are characterized by weak interannual variability.

[Place Figure 27 here]

Different factors are investigated for their relationships with CHL (Figure 28). For example, SST describes the fundamental features of the ocean that can influence the growth rate of phytoplankton and subsequently impact CHL. For the majority of the SCS, there are high correlations between SST and CHL (Figure 829A), and most of the correlations can reach more than -0.8. It is important to point out that high correlation does not indicate causation between these two factors. As SST reached its annual maximum in summer, the MLD became shallowest²¹. Nutrients supplied to the euphotic layer were low because vertical mixing was blocked by intensive stratification¹³. As a result, low nutrients limited the growth rate of phytoplankton and resulted in low CHL. In contrast, high CHL occurred in winter when the MLD was deeper, and low

SST induced weak stratification³⁵.

[Place Figure 28 here]

Wind-driven mixing can be approximately gauged by WS and was used to describe vertical mixing 18. Large correlation coefficients, with values of approximately 0.8, are identified between the WS and CHL levels north of the SCS (Figure 829B), particularly in the regions with the strongest winter wind located on the northern shelf of the SCS. Weak but significant correlations can be found to the south. Correlations between WSC and CHL were significant in the majority of the SCS (Figure 829C), although they showed opposing signs in the north and south. The positive correlation coefficient between CHL and WSC is to the south, and the negative values are in the north. The region between them is characterized by a nonsignificant correlation. The WS and CHL were found to be strongly correlated in the corresponding region where the winter WS was largest.

The front can induce CHL variability, which was investigated here. A large correlation was found in the northeast and southwest of the SCS (Figure 829D). CHL increased as frontal activities became more active³⁶. The SLA showed a significant negative correlation with CHL from the northeast SCS towards the southwest and a positive correlation along the west coast of the SCS (Figure 829E). It is interesting to note that the positive correlations are limited in the region with shallow topography.

[Place Figure 29 here]

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To the northeast of the SCS, all the correlations are prominent (Figure 298). Thus, the correlations of monthly time series between CHL and other parameters are calculated using the spatial average in a designated box (Figure 829A). The results show that most of the factors are intercorrelated with significant correlations (top right section of Table 1). Because the seasonal cycle dominates the time series, the correlation is no longer valid after removing the monthly average (bottom left section of Table 1).

[Place Table 1 here]

[Place Table 1 here]

The correlations in the seasonal cycle are not significant for some regions, e.g., southwest of the SCS (Figure 289). The region is dominated by dynamic processes, e.g., upwelling and wind-induced offshore transport, which determine the variability in CHL¹⁷. A significant correlation between CHL and other factors, e.g., SST, WS, fronts and WSC, was identified in anomalous fields (Figure 309). The anomalies were calculated for the monthly time series by removing the corresponding monthly average. The effective number of degrees of freedom can be increased, but it does not impact the underlying relationships among their time series 28,37.

[Place Figure 30-9 here]

In anomalous fields, CHL and SST were significantly correlated in the majority of the SCS (Figure 930A). When SSTs were anomalously high (low), CHL became anomalously low (high). Similarly, an anomalously high (low) WSC and fronts to the southwest of the SCS can induce a large (weak) CHL (Figure 930C, 930D). In addition, a negative correlation is found between the anomalous SLA and CHL levels (Figure 930E). Different lags were tested, and the correlation only became significant if no lag was deployed; thus, CHL is simultaneously impacted by anomalies in SST, WSC, fronts, and SLA. Their relationship was further investigated using the spatially averaged monthly time series southwest of the SCS (designated as a green box in Figure 930A). The results show that most of the factors are intercorrelated with significant correlations in the anomalous field (bottom left section of Table 2).

[Place Table 2 here]

FIGURE AND TABLE LEGENDS:

Figure 1: Procedure for downloading SST and CHL data from websites, shown as snapshots. A. The website of Po.Daac: B. access the data drive, C. login to the data system, D. locate designated data directory and E. click to download daily data file in nc format.

Figure 2: Screenshot of the procedure to add 'UTILITIES' with subfolders to the Matlab path

Figure 3: Screenshot of the procedure to read the CHL and SST data by running 'Read_MODIS_CHL.m' and 'Read_MODIS_SST.m', respectively.

Figure 4: Screenshot of the procedure to read the SLA data by running 'Read_SLA.m'.

Figure 5: Screenshot of the procedure to read the wind vector data by running 'Read_WindVector.m'.

Figure 6: Screenshot of the procedure to download topography data from websites, which are shown as snapshots. A. The website of the National Oceanic and Atmospheric Administration (NOAA) National Center for Environmental Information: B. select data using the range of longitude and latitude and C. download data in xyz format.

Figure 7: Screenshot of the procedure to read the topography data by running 'Read_topography.m'.

Figure 8: Screenshot of the procedure to replace the original SST and CHL data with 3 day average data using 'Temporal_average.m'.

Figure 9: Screenshot of the procedure to interpolate 3-day averaged SST and CHL into the same grid as the wind data.

Figure 10: Screenshot of the procedure to calculate the wind stress curl using

571 'Wind stress curl.m'. 572 573 Figure 11: Screenshot of the procedure to the calculated time series of monthly averaged SST 574 and CHL using 'Monthly_average.m'. 575 576 Figure 12: Screenshot of the procedure to smooth 3-day average SST data spatially using 577 'Spatial smoothing.m'. 578 579 Figure 13: Screenshot of the procedure to obtain the SST gradient vector using 580 'SST_gradient.m'. 581 582 Figure 14: Screenshot of the procedure to identify the front as the local maximum and suppress pixels with a gradient less than 90% of the maximum using 'Local_maximum.m'. 583 584 585 Figure 15: Screenshot of the procedure to calculate the monthly frontal probability using 586 'Monthly_FP.m'. 587 588 Figure 16: Screenshot of the procedure to decompose monthly time series using 589 'Empirical_orthogonal_function.m' for different variables to obtain spatial and temporal 590 variability. 'Amp' is the amplitude, 'Mag' is the magnitude, and 'Eig' is the Eigen values for 591 different modes. 592 593 Figure 17: Screenshot of the procedure to calculate seasonal correlation using monthly time 594 series of different variables via 'Seasonal_correlation.m'. 595 596 Figure 18: Screenshot of the procedure to calculate anomalous correlation using monthly time 597 series of different variables via 'Anomalous_correlation.m'. 598 599 Figure 19: Screenshot of the procedure to produce Figures 20, 21, 22 and 25. 600 601 Figure 120: Original observations for major parameters on April 15, 2015. A. Chlorophyll (CHL), 602 B. sea surface temperature (SST), C. wind stress curl (WSC) with wind stress (WS) vector, D. sea 603 surface anomaly and **E.** topography for the ocean basin. 604 605 Figure 24: Sea surface temperature (SST) for a single day on April 15, 2015. A. Original SST from 606 MODIS, B. three-day averaged SST and C. SST after spatial smoothing. 607 608 Figure 322: Procedure for front detection derived from SST. A. Magnitude of SST gradient, B. 609 the distribution of the SST front in thin black color and C. front distribution with the 610 corresponding SST. 611 612 Figure 423: Monthly average for major parameters in April 2015. A. CHL (in logarithm scale), B. 613 SST, C. wind stress curl (WSC) with wind stress (WS) vector, D. sea surface anomaly and E. frontal

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probability (FP).

Figure 24: Screenshot of the procedure to produce Figures 25, 26 and 27.

Figure 25: The EOF for CHL. A. Magnitude of EOF1, B. magnitude of EOF2, C. monthly averaged time series of EOF1, D. monthly average for EOF2 and E. monthly time series of EOF1 (black) and EOF2 (blue).

Figure 26: Same as in Figure 25 but for SST.

Figure 27: Same as in Figure 25 but for FP.

Figure 28: Screenshot of the procedure to produce Figures 29 and 30.

Figure 298: Correlations between CHL and other factors at the seasonal scale. A. SST, B. wind stress (WS), C. wind stress curl (WSC), D. frontal probability (FP) and E. sea level anomaly (SLA). The gray color indicates that the correlation is nonsignificant. Spatially averaged variables are calculated based on the green box in the left panel. Their time series are used to obtain the correlation coefficients in Table 1. This figure has been modified from Yu et al. (2019)¹⁷.

Figure 309: Correlation between CHL and other factors in the anomalous field. A. SST, B. WS, C. WSC, D. FP and E. SLA. The gray color indicates that the correlation is nonsignificant. Spatially averaged variables are calculated based on the green box in the left panel. Their time series are used to obtain the correlation coefficients shown in Table 2. This figure has been modified from Yu et al. (2019)¹⁷.

Table 1. Correlation coefficients of the time series among factors, located northeast of the SCS, e.g., SST (sea surface temperature), FP (frontal probability), WSC (wind stress curl) and WS (wind stress), using the box shown in Figure 11A. The monthly average and anomaly top are shown in the top right section and left bottom section, respectively. Red fonts indicate that the correlation cannot fulfill the 95% confidence level. The table has been modified from Yu et al. (2019)¹⁷.

Table 2. Similar to Table 1 but for correlation coefficients of anomalous time series in the southwest SCS (see Figure 12A for location). The table has been modified from Yu et al. (2019)¹⁷.

DISCUSSION:

In this study, the major features of marine systems are described using satellite observations. The CHL, which can be used to represent ocean production, is selected as an indicator factor. Factors related to CHL variability were investigated using monthly averaged time series, e.g., SST, WS, WSC, FP and SLA. Three critical steps are described in this study: acquiring satellite data for different parameters, describing their spatial and temporal variabilities via EOF, and determining interrelationships among different factors by calculating correlation coefficients. A detailed procedure showing the identification for daily frontal distribution, which is derived from the SST observations, is included. Two major approaches have been developed for SST front detection: the gradient method^{10,38} and the histogram method^{39,40}. The histogram method is based on a

similar range of values for SST, which can be used to divide the water masses into different groups. The pixels with values between different groups representing the pixel in a transitional band are defined as fronts. On the other hand, the gradient method separates several relatively uniform water bodies as pixels with large gradient values. A comparison study was conducted, and they found lower false rates using the histogram method and fewer missed fronts using the gradient method⁴¹. In this study, the gradient-based method³⁸ was adopted following former studies^{10,28}. The algorithm can avoid front break-up into multiple edge fragments by allowing the magnitude to decrease to a level below a smaller threshold. In addition to the dataset included here, other satellite observations, such as the aerosol index, can also be used with a similar approach.

Most of the procedures can be directly applied in other regions or datasets. Modification may take place to change the threshold of front detection. Because the SST gradient in the SCS is comparable with the Eastern Boundary Current System²⁸, the same thresholds were implemented for the current study. A previous study revealed that the SST gradient from different datasets can vary as much as three times⁴², which makes the method somehow less objective. Substantial studies have investigated frontal activities around the global oceans^{28,43}. The best approach to validate fronts is to compare them with in situ observations. Yao⁴⁴ described the monthly frontal distribution for the SCS. Their results agreed well with the in situ measurements. The overall gradient should be checked and adjusted since its value may vary depending on the spatial resolution and instruments. In particular, the threshold should be updated when another SST dataset is used. A basic understanding of the regional dynamics is fundamental to understanding frontogenesis^{45,46,47}. The front detection script can be developed by individual authors based on the description in this paper.

Satellite information offers a comprehensive understanding of surface features, and a results comparison with in situ observations can aid in evaluating credibility. However, satellite observations are limited to the ocean surface, which limits the application for understanding the vertical structure of the water column. In a recent study, satellite observations revealed that the surface CHL increased by 15 times, but the vertical integrated value only increased by 2.5 times⁴⁸. This difference was because the surface value was impacted by the coeffects of phytoplankton growth and shoaling of MLD, resulting in an unrealizable value at the surface. Thus, the surface feature may not offer an accurate description for the entire water column. Additionally, the influence of cloud coverage limits the continuous observations of satellites. Thus, monthly time series are calculated for different factors over the same region and same period. This will guarantee the credibility of calculating the correlations among different factors. However, the short-period events, e.g., typhoons that last for a few days to a week, will not be resolved.

Compared with former studies, the proposed method can offer spatial information at the pixel level, which can help to evaluate the dynamics in a more detailed manner. Some former studies averaged the entire SCS as a single number and obtained a time series. They found that an unusually strong WS and high SST can induce anomalously high CHL¹⁶, which is consistent with current result. However, the spatial variation in the relationships was not resolved. In this study, the basin-scale correlation between WS and CHL was weak in the anomalous field. A large

significant correlation was only identified for certain areas, e.g., in the center of the SCS (Figure 32B). Thus, the current method offers a comprehensive description for investigating spatial variations. Similarly, observations from two Bio-Argo floats were used and revealed that WSC did not correlate with CHL variability²⁰. However, the trajectories of the two floats are only located in certain regions. In this case, it was exactly within the band where the correlation between the CHL level and the WSC was not significant (Figure 31D). The proposed method is very helpful for resolving the spatial dependence among factors, which is a fundamental characteristic of the global ocean.

In summary, the method used here can accurately describe the spatial distribution and temporal variability in ocean surface features using satellite observations. With the increasing resolution of satellite datasets, more detailed features can be identified and investigated, which enables a general understanding of regional features, including CHL, SST, and SSH. The correlation of monthly time series among different factors can aid in understanding their dynamic relationships and potential impact on an ecosystem⁴⁹. Because the correlation can largely vary at different spatial locations, the proposed method offers a detailed and comprehensive description. A similar approach can be applied to any ocean basin worldwide, which will be greatly helpful to improve the understanding of marine dynamics and ecosystems.

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The authors have nothing to disclose.

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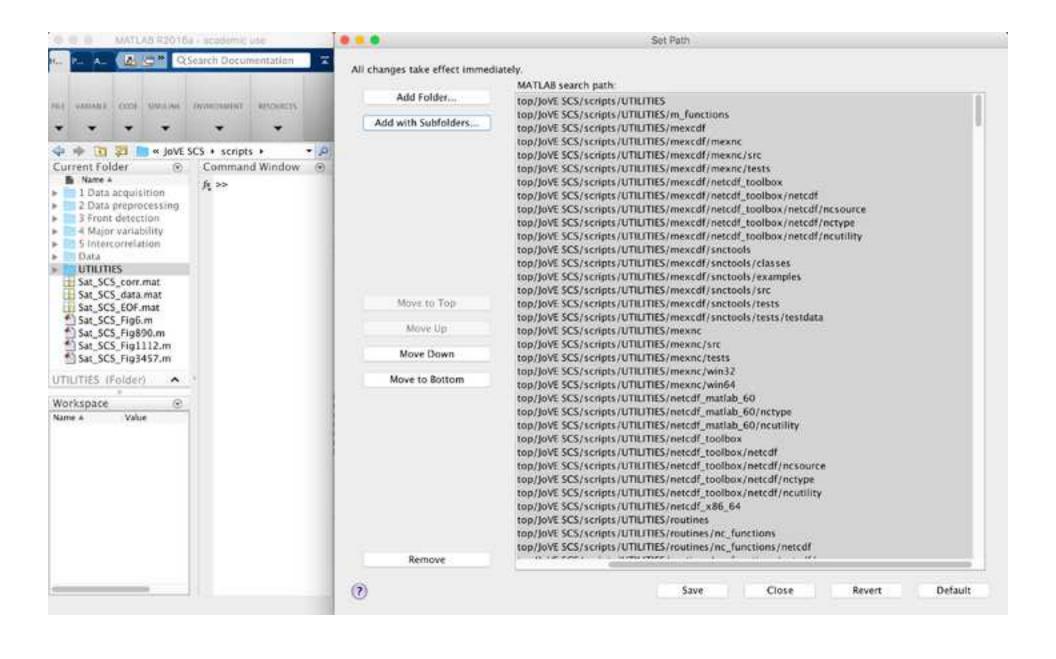


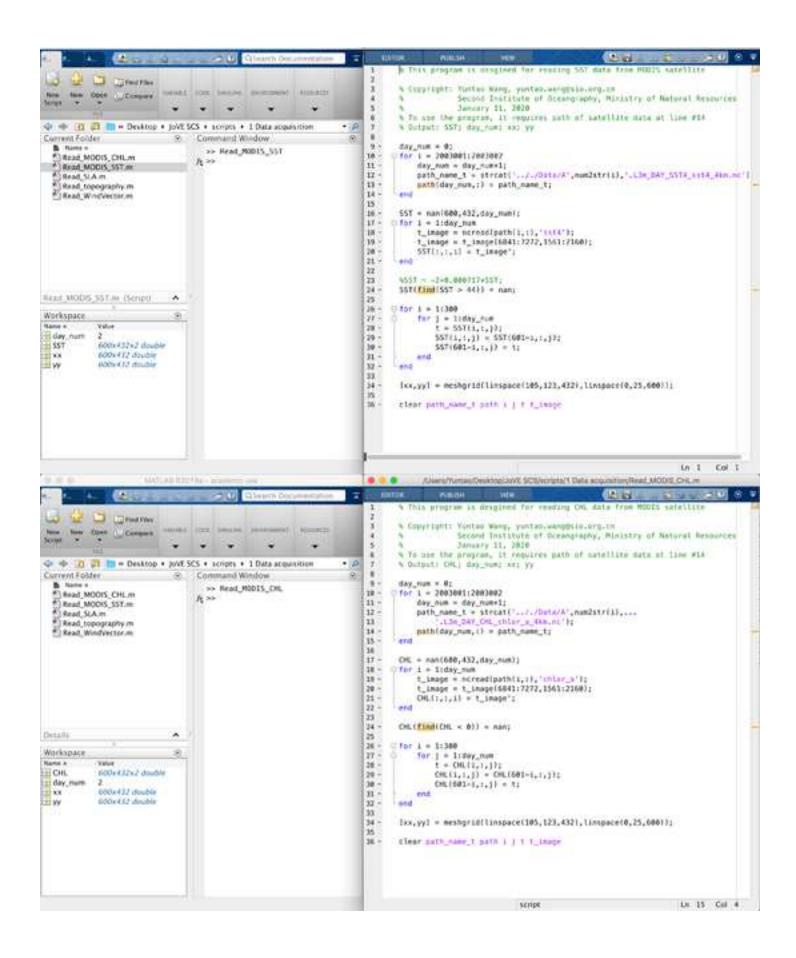


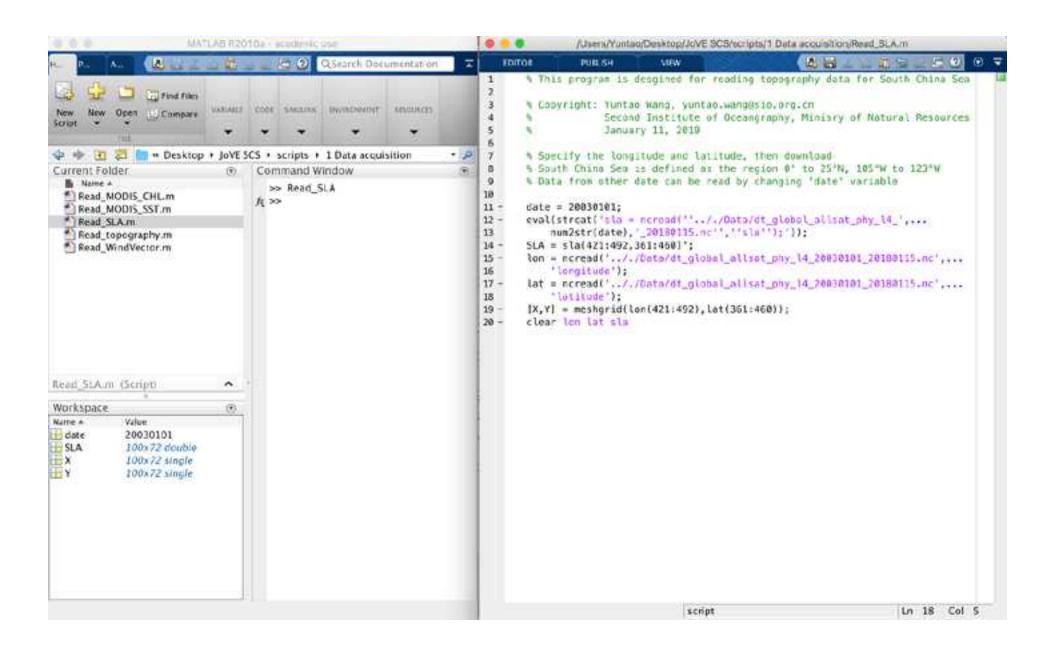


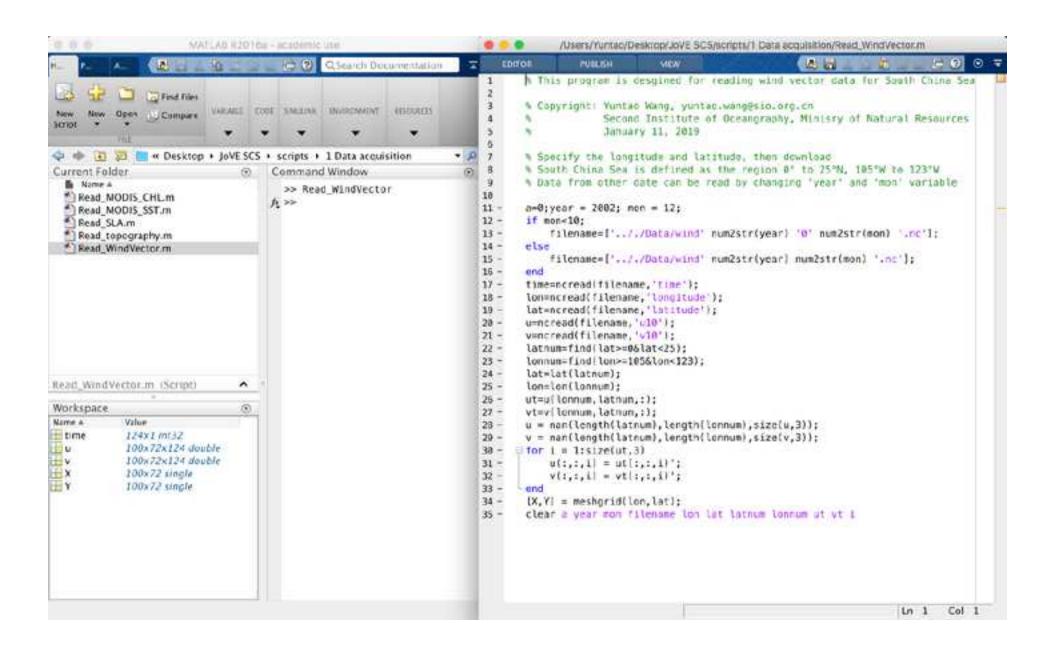


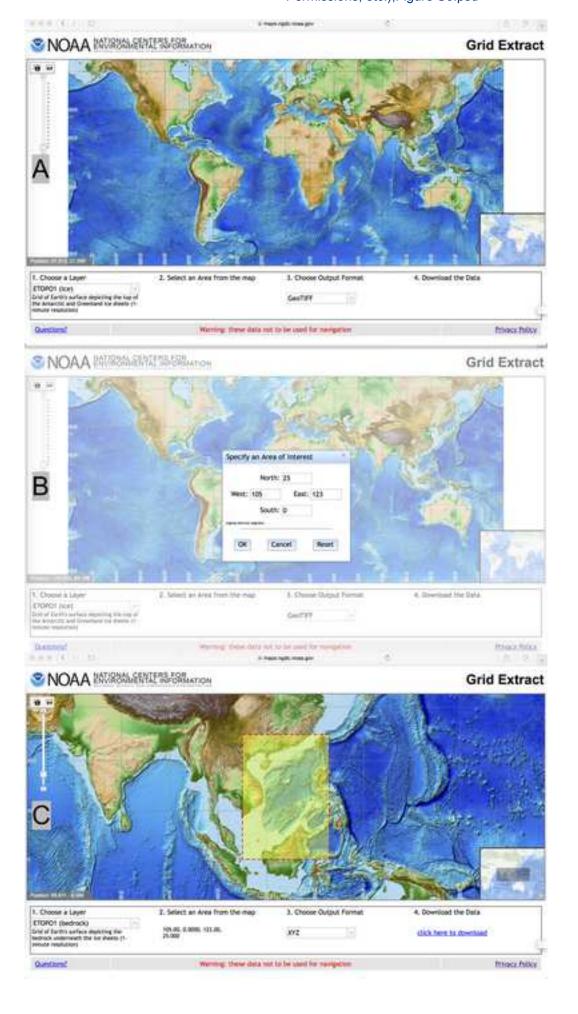


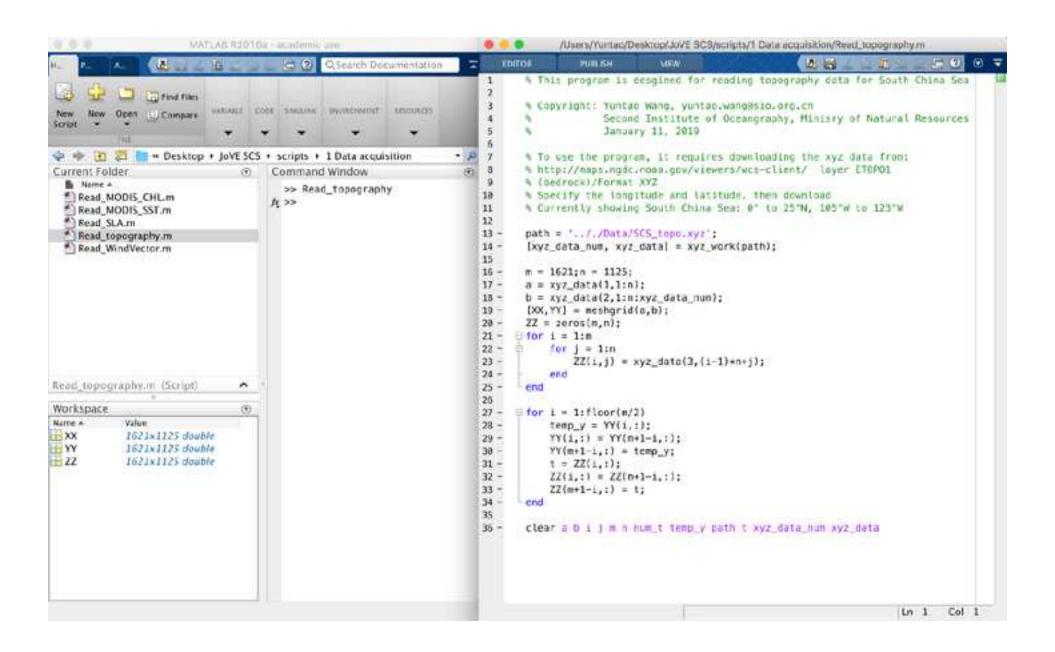


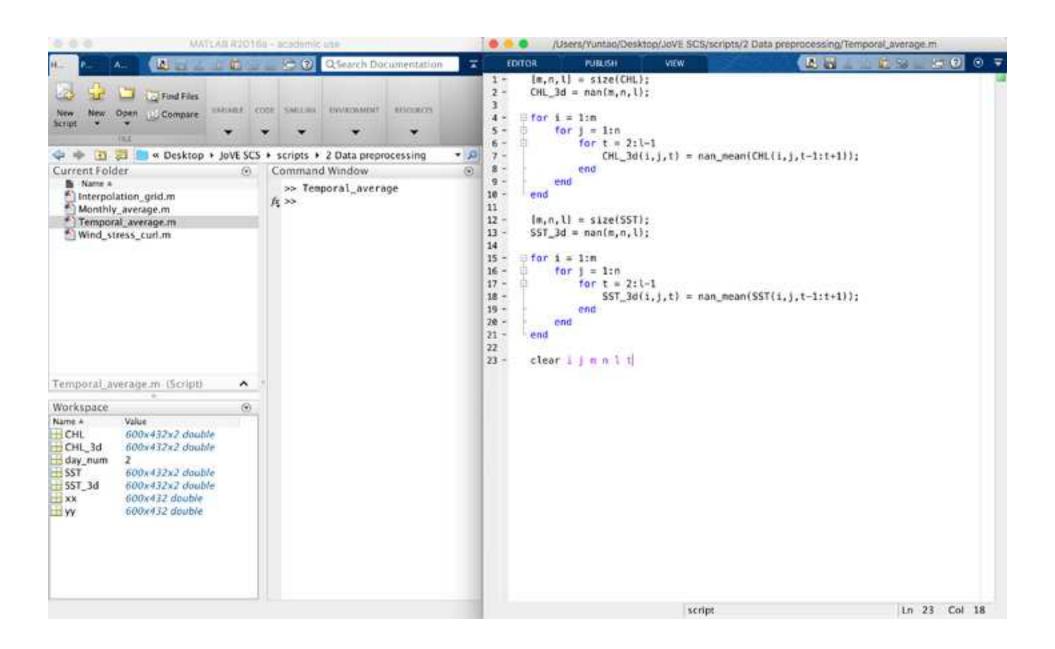


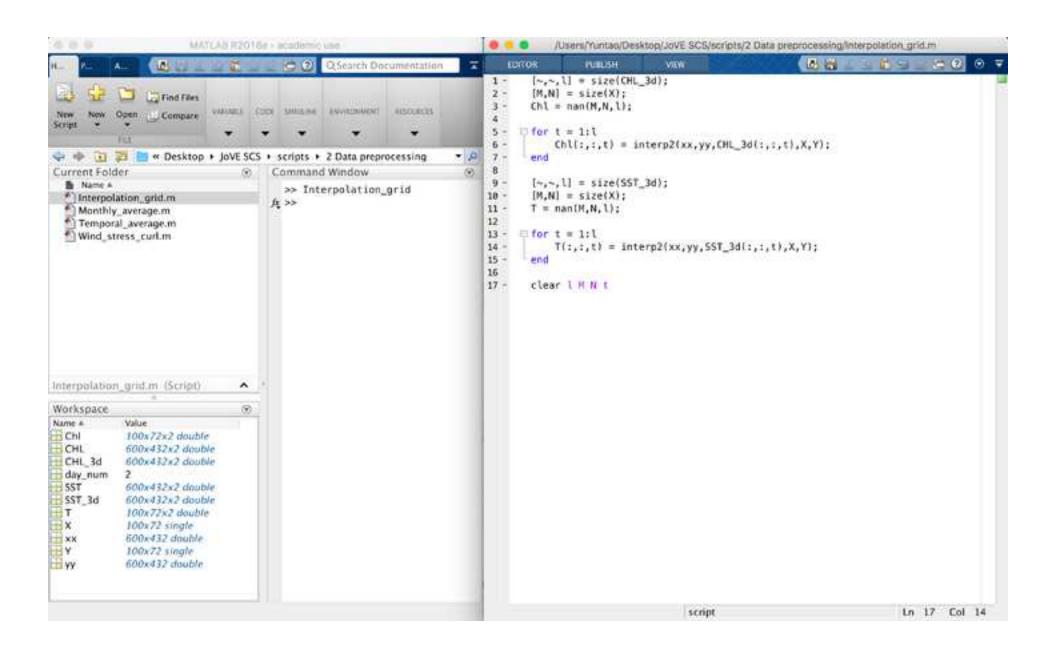


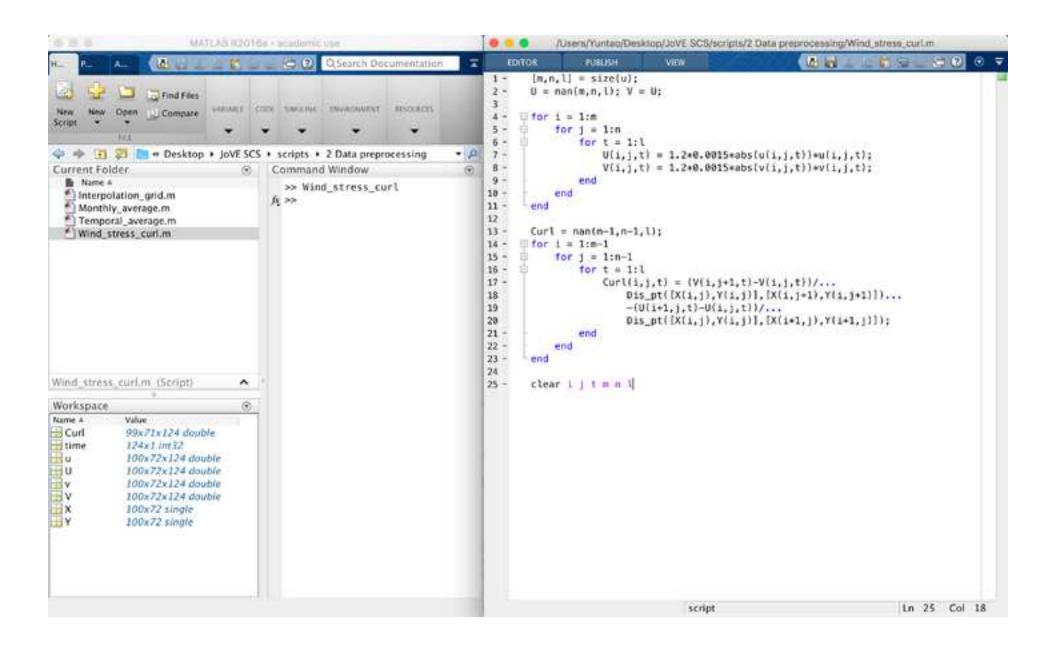


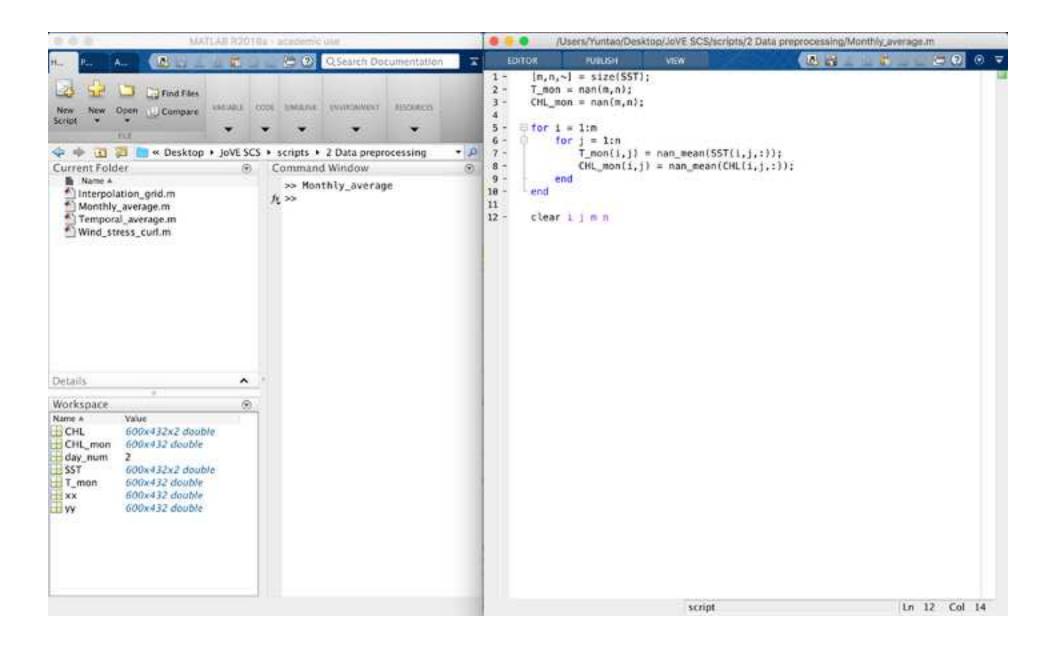


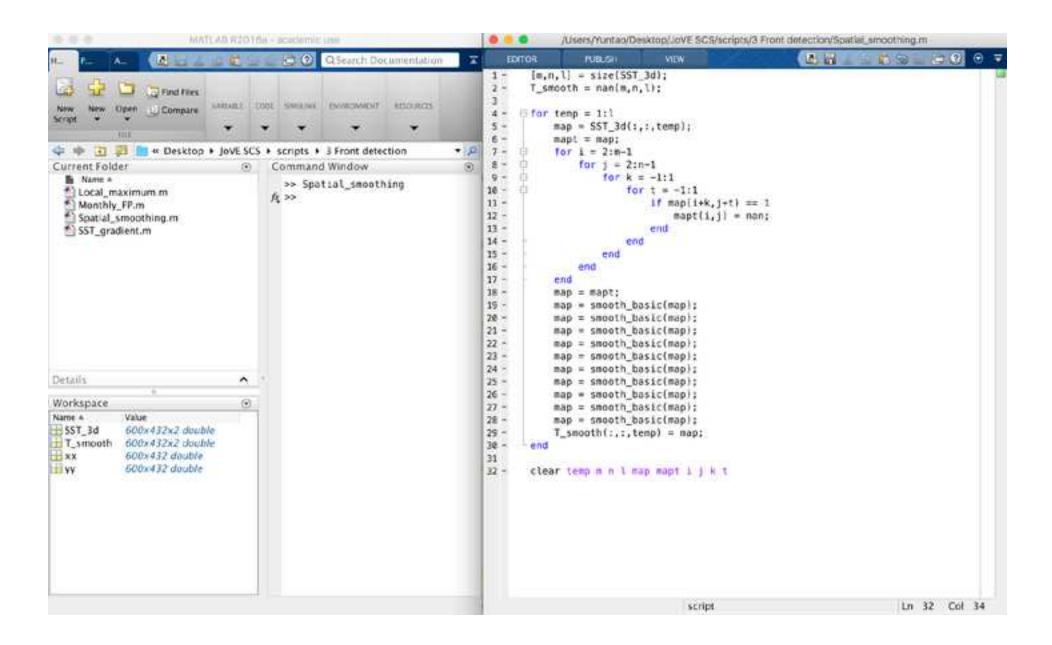


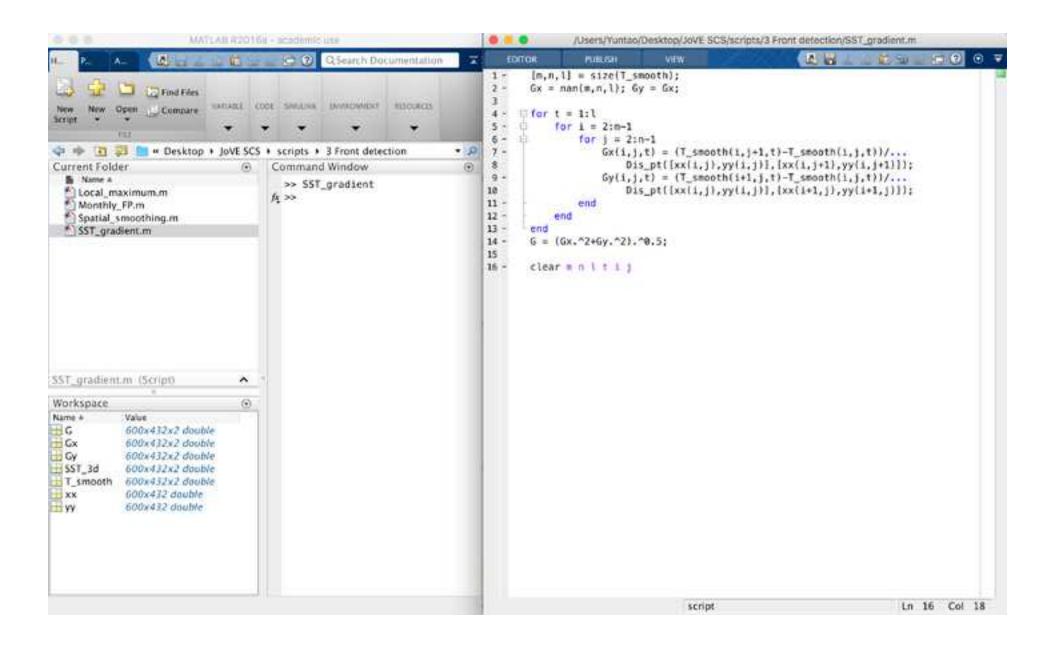


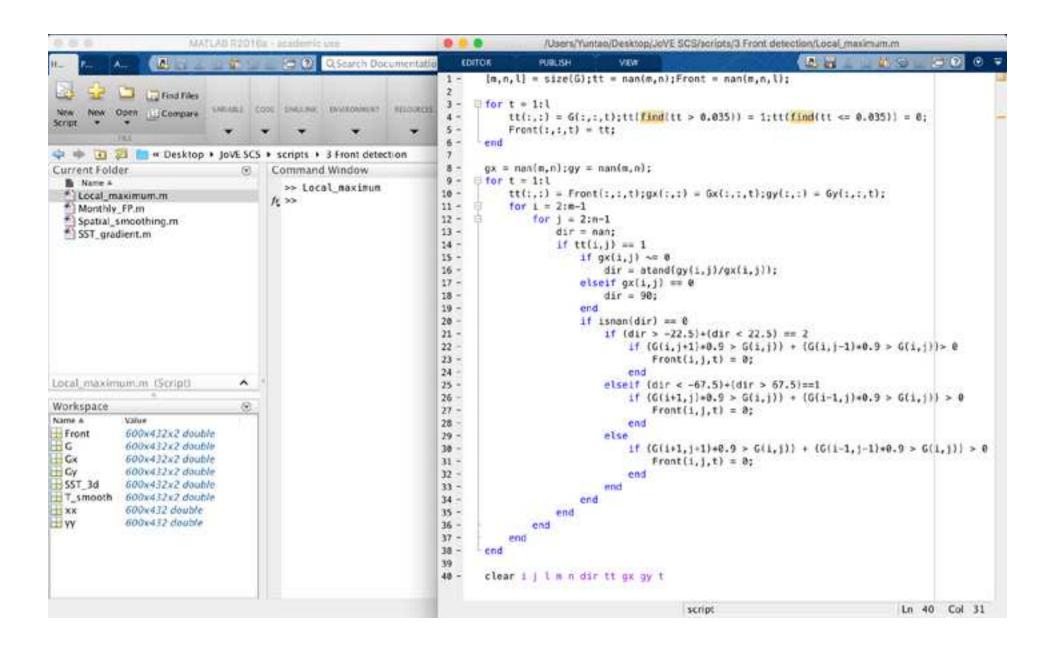


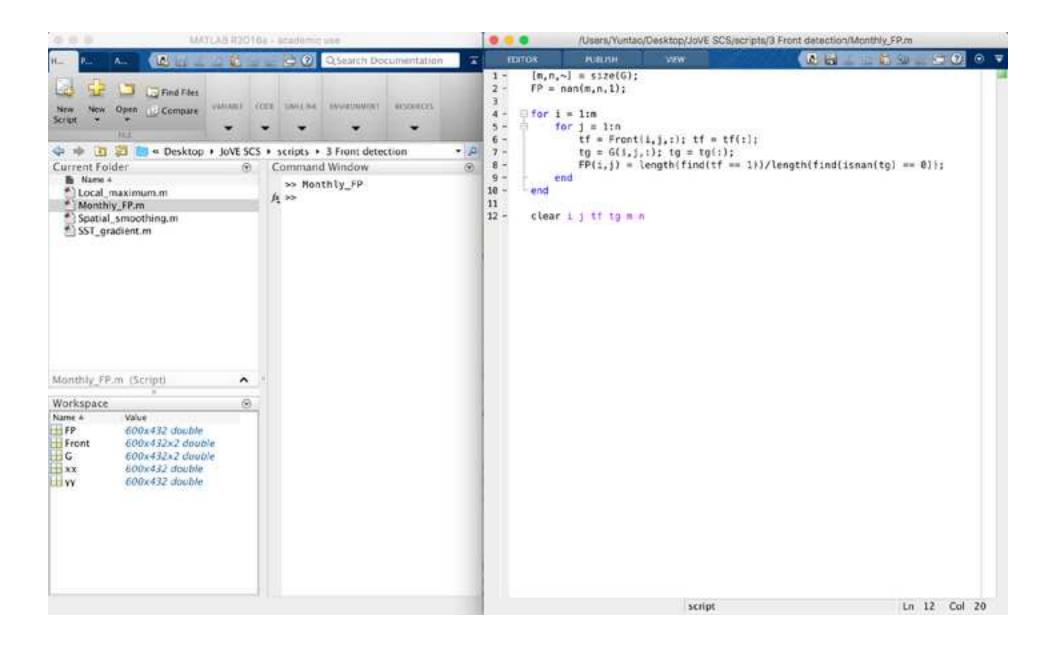


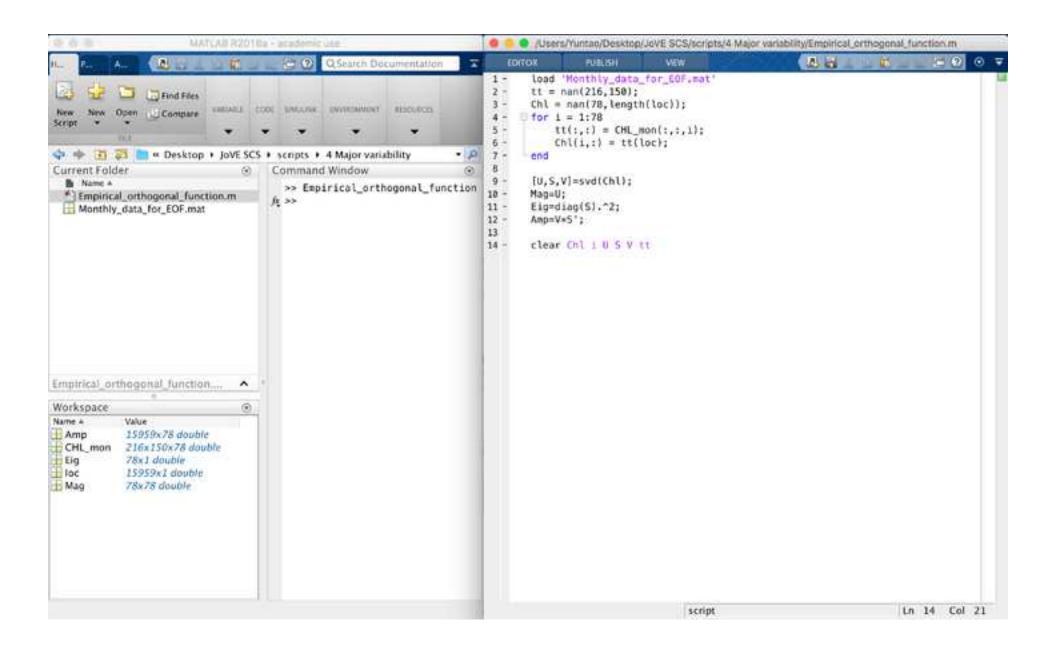


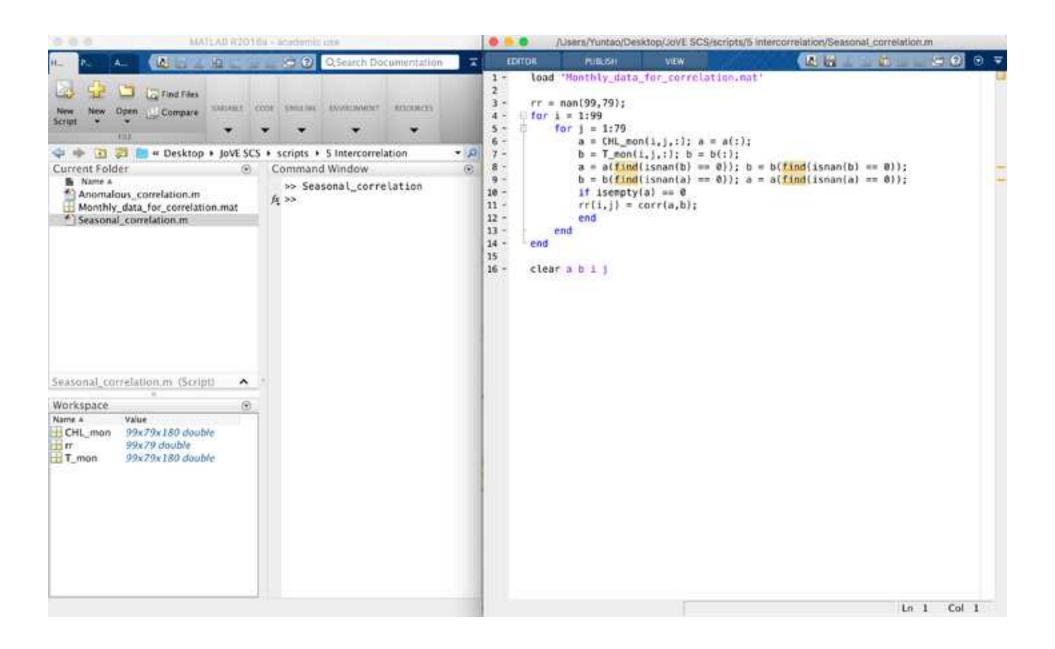


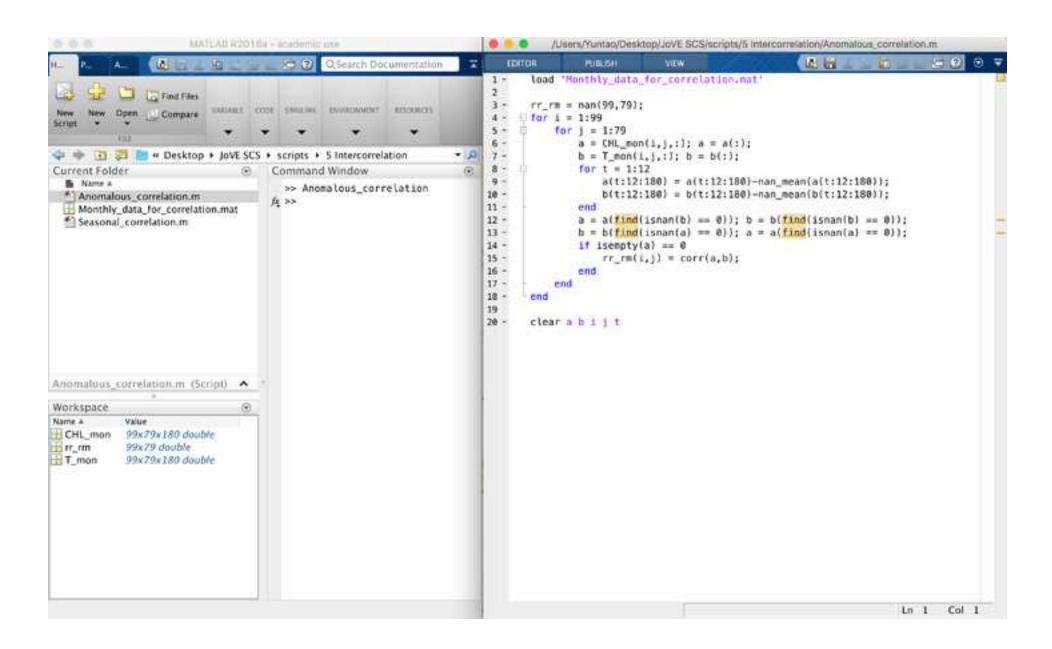


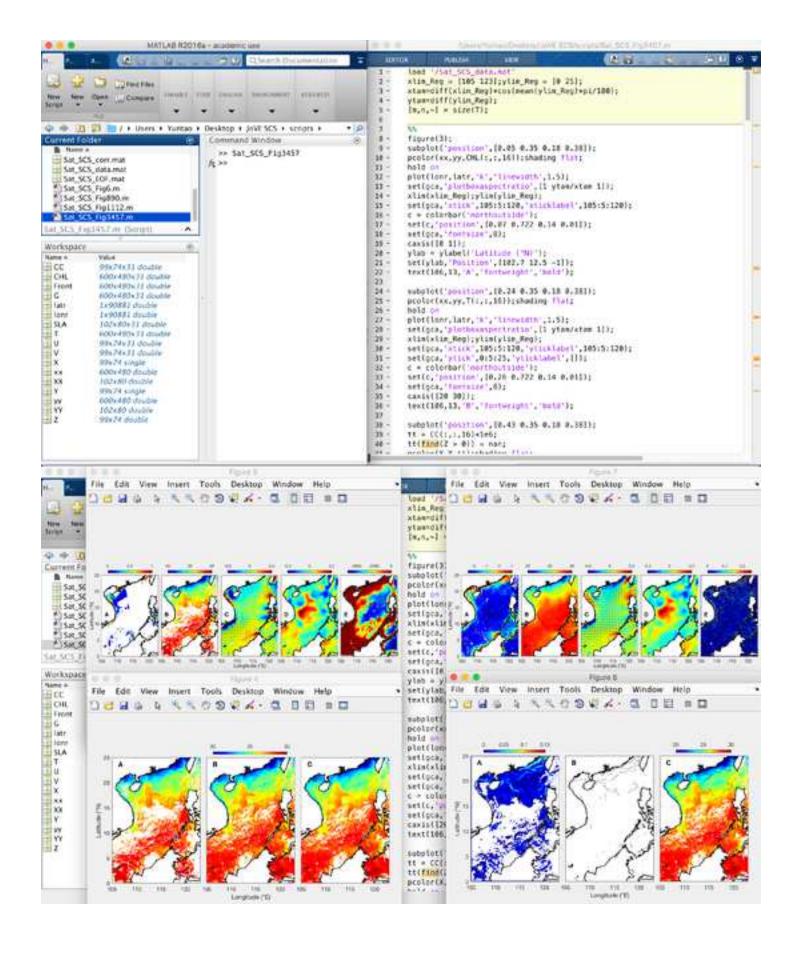


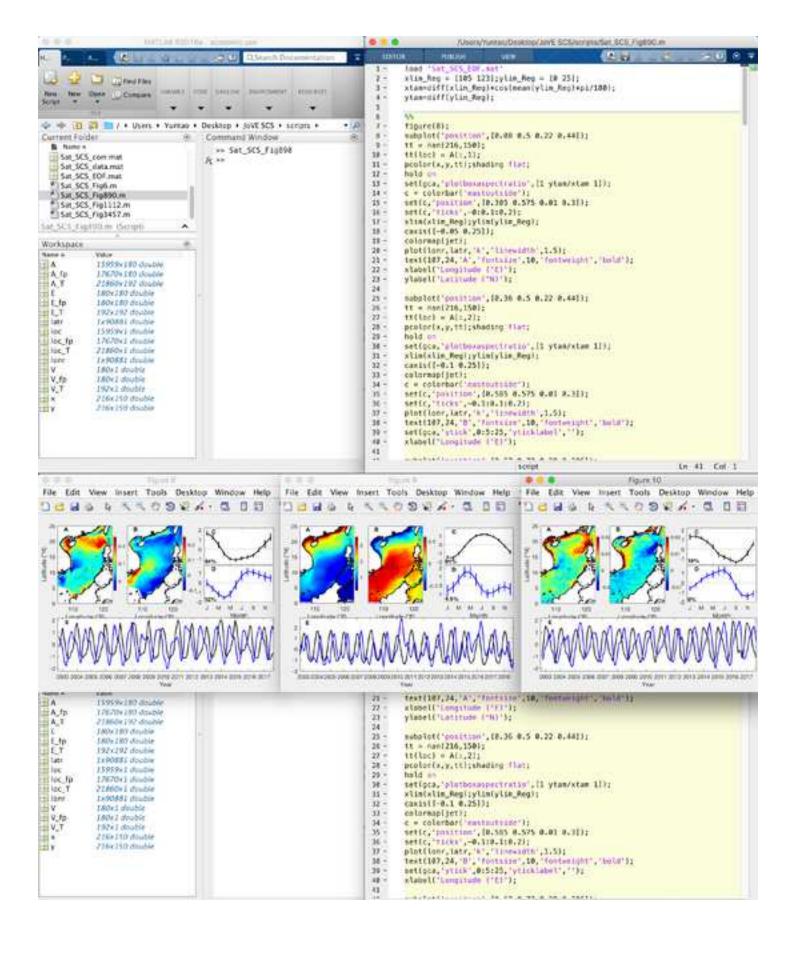


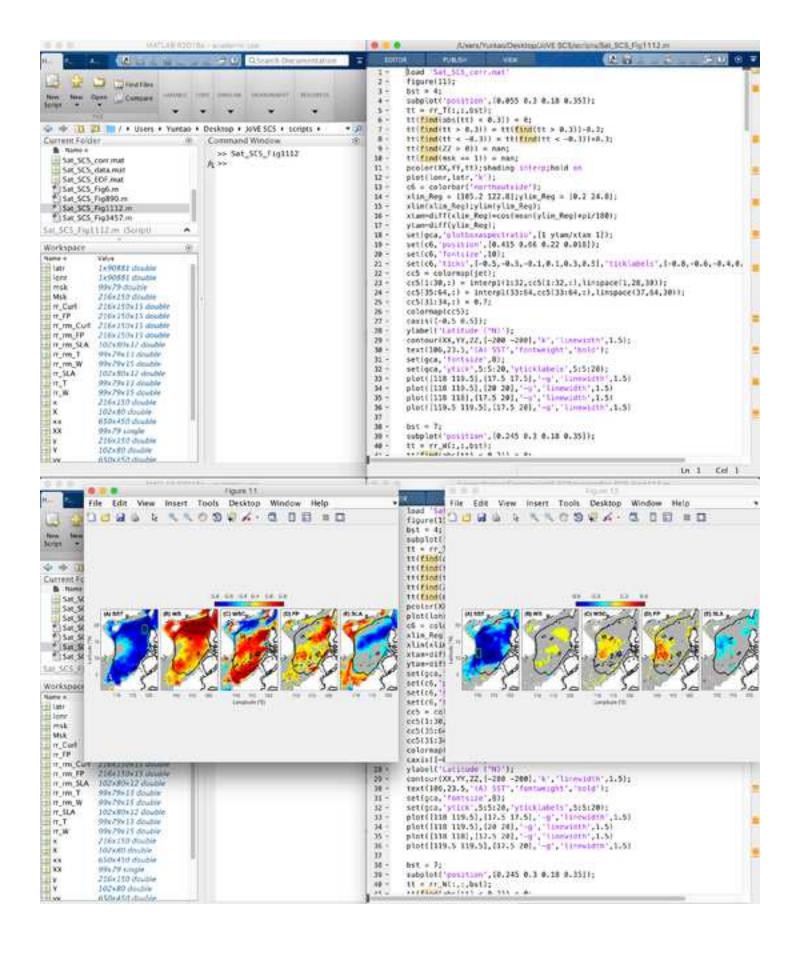












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