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Feasibility of an open-source algorithm for predicting sea surface temperature based on three multi-resolution data sources

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The utilization of space borne platforms for the quantification of Sea Surface Temperature (SST) has brought about a major shift in the collection of global information. However, the acquisition of SST through satellite images is limited by its coarse spatial resolution. To address this issue, downscaling algorithms can be implemented to generate matrices with higher spatial resolution. Current research used the SST data source from the MODIS-Aqua sensor at three distinct spatial resolutions of 9 km, 4.5 km, and 1 km in the Gulf of California, Mexico. The original SST images were then downscaled to 4.5 km, 1 km, 500 m, 250 m, and 125 m per pixel scales using an open-source algorithm. Results indicate a robust linear correlation between the original SST-MODIS data and the modelled data for all spatial resolutions. This study demonstrates the feasibility of utilizing an open-source downscaling algorithm to enhance the spatial resolution of SST images in a marginal sea.

[**Keywords**: Downscaling, Gulf of California, Sub-pixel mapping, Super-resolution mapping]

Introduction

Remote sensing has emerged as a viable alternative for gathering instantaneous data in large-scale studies. However, the accuracy of remote sensing data is generally lower compared to *in situ* measurements, and sensors involved may only capture data from the surface layer of the sea[1]. Despite this limitation, satellite observations offer a wide range of spatial and temporal resolutions that largely offset this drawback. It is well known that *in situ* measurements have been valuable complementary means to validate satellite data[2] and improve the quality of remote sensing data[3]; but they may not be feasible in some inaccessible locations. Therefore, space borne observations remain the only available data source[4].

Remote sensing, geographic information systems, and modelling techniques have proven to be highly effective tools in numerous studies aimed at monitoring coastal and oceanic systems[5,6]. Satellite data can be used to estimate various variables and among them, Sea Surface Temperature (SST) has been widely employed in large-scale oceanographic studies[7]. SST plays a critical role in the exchange of energy between the ocean and atmosphere interface[8], making it an essential variable for analyzing climate change[9]. Furthermore, it is a valuable parameter for assessing various oceanographic phenomena such as the direction and forecast of tropical storms and hurricanes, identifying areas with high turbulent kinetic energy[10], evaluating dynamic biogeographic regions[11], determining the influence of suspended terrestrial sediment from rivers[12], and detecting the potential impacts of the El Niño Southern Oscillation (ENSO) event. Additionally, the spatial variability of SST has been linked to the strengthening of the density gradient, leading to a reduction in the transport of nutrients through the pycnocline[13], which has been quantified using thermal infrared bands since the early 1980s[14].

The spatial resolution of an image refers to the number of pixels used to create it, which determines the amount of information that can be obtained from that image. As a rule, images with higher spatial resolution provide greater detail and information[15]. However, creating gap-free reconstructions of remote sensing data has long been a challenge. Therefore, interpolation algorithms have often been employed to fill in these gaps[16,17]. One potential solution to this problem involves the use of downscaling techniques, which can provide spatial information at a higher level. These techniques include transforming the original image data into matrix sequences with finer spatial resolutions[18]. In essence, downscaling functions by treating pixels as a combination of surrounding pixels that affect a central one based on their linear distance[19]. As such, this allows

for the estimation of higher-resolution indicator values from lower-resolution fractional values[20] without prior spatial knowledge[18].

The purpose of this study was to examine an open-source downscaling technique implemented along the Gulf of California (GC) in Mexico to enhance the spatial resolution of SST satellite data. The main objective of the study is to assess the effectiveness of a downscaling algorithm that utilizes the same MODIS-Aqua data source with spatial resolutions of 9 km, 4.5 km, and 1 km. Specifically, to generate SST data maps with pixel reductions of 4.5 km, 1 km, 500 m, 250 m, and 125 m while linking these data to SST algorithms in coastal and ocean waters through 1-by-1 and 3-by-3-pixel sampling areas.

Materials and Methods

Study area

Situated on the northwest coast of Mexico, the GC is a long and narrow marginal sea that extends over 1000 km in length with a variable width of approximately 90–200 km, encompassing both marine and terrestrial regions over a total area of 265900 km^2 (Fig. 1). Its distinctive geomorphology and wind-driven processes induce strong vertical currents, resulting in upwelling of dissolved nutrients towards the surface, which in turn leads to elevated primary productivity[21]. Despite strong events such as ENSO, the GC maintains its productivity levels[22]. Over much of the year, the distribution of primary productivity indicates a latitudinal gradient, with the highest values in the north and the lowest in the south[2].

Methodology and data analyses

Three SST images were obtained from the MODIS-Aqua sensor on March 2, 2018, with varying initial spatial resolutions of 9 km, 4.5 km, and 1 km. The MODIS-Aqua sensor could capture images daily; however, to ensure optimal image quality, a cloudless day within the Gulf of California was deliberately selected. The images were acquired from the NASA Ocean Colour website (https://oceancolor.gsfc.nasa.gov). The MODIS-Aqua images with 9 and 4.5 km spatial resolution were downloaded at level 3 using an

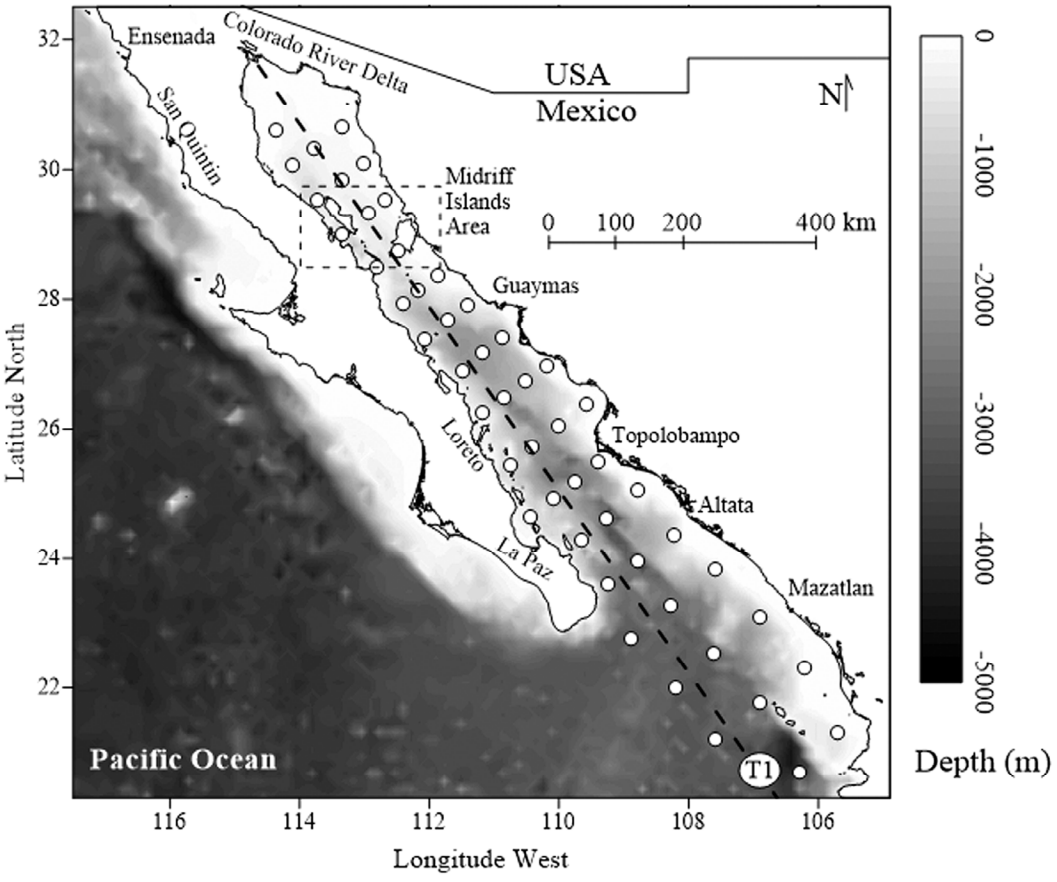

Fig. 1 — Gulf of California bathymetry (m). White circles represent the locations of the 50 stations, and the dashed line is the 1000 km transect (T1)

equidistant cylindrical projection. In comparison, the image with a spatial resolution of 1 km was downloaded at level 2 and then geographically projected at level 3 using the Sea DAS-NASA v7.5.1 program. The geographic boundary of images was restricted from 20.5° to 32° north latitude and 105° to 117.5° west longitude. The Sea DAS software produced three distinct end products with varying spatial resolution and projection. Each end product was tested and analyzed independently using an open-source algorithm. Upon completion of the downscale process, the result obtained will not directly correspond to the original data set, regardless of spatial resolution.

Sea surface temperature level 3 products were generated by combining data from all level 2 products, which were collected over a 24-hours, encompassing both daytime and night-time overpasses, using the SST4 algorithm. It is worth noting that, irrespective of the spatial resolution at which the level 2 products were projected, the SST level 3 products were derived solely from level 2 data. The rationale for using a single day to obtain specific fluctuations in SST is to minimize the inherent smoothing that occurs when averaging a series of daily images (*e.g.*, every eight days or monthly). The level 3 products were designed to replicate the images on a downscale to establish if the spatial patterns are consistent.

An open-source program in R was utilised to process the three SST MODIS-Aqua images and imported the images along with the ncdf4 and raster libraries, which are required to access and view these files. The approach involved using a unique disaggregation factor for each level of processing. For example, matrix M_1 represents four SST pixels at an initial spatial resolution of 9 km:

$$M_1 = \begin{bmatrix} TSM_{i,j} & TSM_{i+1,j} \\ TSM_{i,j+1} & TSM_{i+1,j+1} \end{bmatrix}$$

Where, i and j represent the latitude and longitude positions of the four pixels.

The processing was initiated by downscaling matrix M_1 to a processing level of 4.5 km per pixel using a two-stage method. The initial stage involved downscaling along the horizontal axis (*i.e.*, longitude), followed by the second stage, which involves downscaling between the intermediate values acquired in the first stage but along the vertical axis (*i.e.*, latitude) by means of the following equations:

$$U_{\alpha 0} = [1-\alpha]\, U_{i,j} + \alpha\, [U_{i+1,j}] \quad \ldots (1)$$

$$U_{\alpha 1} = [1-\alpha]\, U_{i,j+1} + \alpha\, [U_{i+1,j+1}] \quad \ldots (2)$$

$$TSM_{x,y} = [1-\beta]\, U_{\alpha 0} + \beta\, [U_{\alpha 1}] \quad \ldots (3)$$

Where, α and β represent the increase in longitude and latitude, respectively; $U_{i,j}$ is the previous SST value located at higher latitude; $U_{i+1,j}$ is the posterior SST value at an upper latitude; $U_{i,j+1}$ is the previous SST value at a lower latitude; $U_{i+1,j+1}$ is the posterior value at a lower latitude, and $TSM_{x,y}$ represents the SST downscaled value with x, y coordinates.

The two previous stages produce a global scale reduction of the values of the matrix M_1 (9 km per pixel) to a new matrix M_2 of 4.5 km per pixel:

$$M_2 = \begin{bmatrix} SST_{i,j} & SST_{i+0.25,j} & SST_{i+0.75,j} & SST_{i+1,j} \\ SST_{i,j+0.25} & SST_{i+0.25,j+0.25} & SST_{i+0.75,j+0.25} & SST_{i+1,j+0.25} \\ SST_{i,j+0.75} & SST_{i+0.25,j+0.75} & SST_{i+0.75,j+0.75} & SST_{i+1,j+0.75} \\ SST_{i,j+1} & SST_{i+0.25,j+1} & SST_{i+0.75,j+1} & SST_{i+1,j+1} \end{bmatrix}$$

The original data set was initially characterized by a spatial resolution of 9 km. However, subsequent steps were undertaken to enhance the quality of the data by reducing its spatial resolution to 4.5 km, 1 km, 500 m, 250 m, and 125 m, thereby generating new data sets with improved spatial resolutions. Similarly, the SST data, which had a resolution of 4.5 km, was also subjected to the same procedure, resulting in data sets with better spatial resolutions of 1 km, 500 m, 250 m, and 125 m. Furthermore, the SST data with a spatial resolution of 1 km underwent further manipulation, producing matrices with even better spatial resolutions of 500 m, 250 m, and 125 m (Fig. 2).

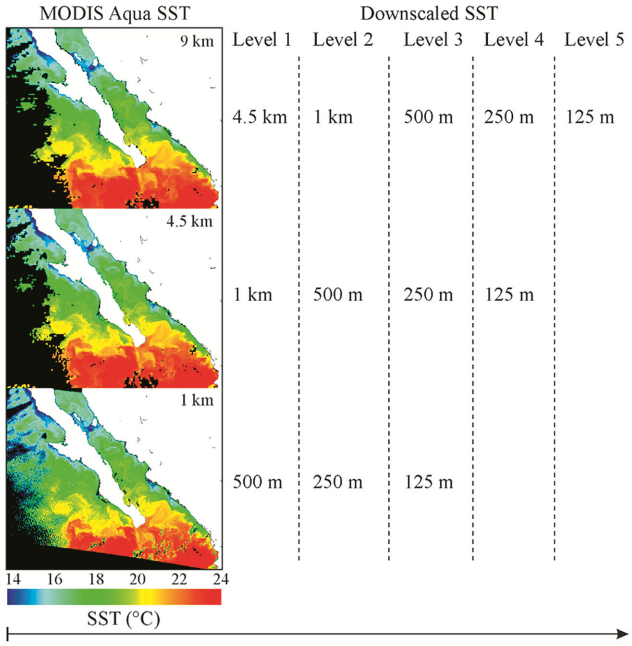

Fig. 2 — Flowchart diagram of the downscaled analysis with MODIS-Aqua data through an open-source approach

Each data set was compared quantitatively by collecting SST values using two distinct sampling methods, 1-by-1 and 3-by-3-pixel sampling areas, at 50 randomized stations throughout the GC. Following this, the mean SST value for each sampling area was calculated as per the methodology outlined in Loisel[6]. In addition, SST data was collected along a 1000 km longitudinal transect throughout the GC. The SST spatial pattern within the Midriff Islands area was visually inspected using the original MODIS and downscaled images. This area was selected due to the strong SST gradient and intense tidal mixing, with an amplitude of approximately 5 m.

The linear association between the downscaled SST values and the original MODIS-Aqua data sets was analyzed using the coefficient of determination (R^2) and the *F*-test of Analysis of Variance (ANOVA). Linear analysis was performed using SST data extracted from 1-by-1 and 3-by-3-pixel sampling areas.

Results

The diagram in Figure 3 shows the linear regression results between the original MODIS sensor SST values and the downscaled SST data, utilizing 1-by-1 and 3-by-3-pixel sampling areas. The study compared the 4.5 km SST MODIS image and the 4.5 km downscaled image extracted from the 9 km MODIS data. A similar comparison was made between the 1 km MODIS image and the 1 km

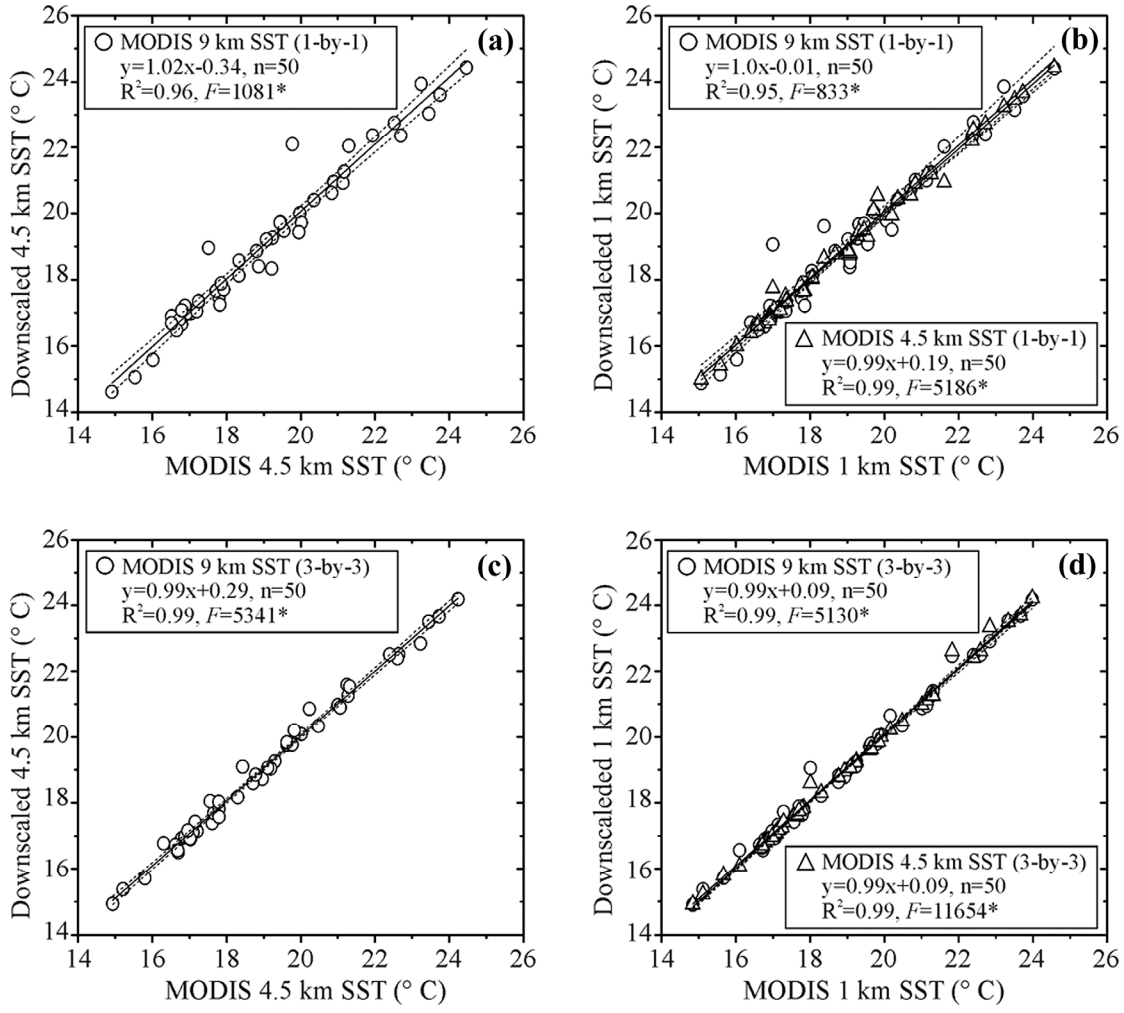

Fig. 3 — Linear regressions between MODIS Sea Surface Temperature (SST) and downscaled SST based on an open-source algorithm. (a) MODIS 4 km data versus downscaled 4.5 km data from the MODIS 9 km data (1-by-1 pixel size), (b) MODIS 1 km data versus downscaled 1 km data from the MODIS 9 km and 4.5 km data (1-by-1 pixel size), (c) MODIS 4.5 km data versus downscaled 4.5 km data from the MODIS 9 km data (3-by-3-pixel size), and (d) MODIS 1 km data versus downscaled 1 km data from the MODIS 9 km and 4.5 km data (3-by-3-pixel size). Asterisks indicate significant *F* values at $\alpha = 0.05$

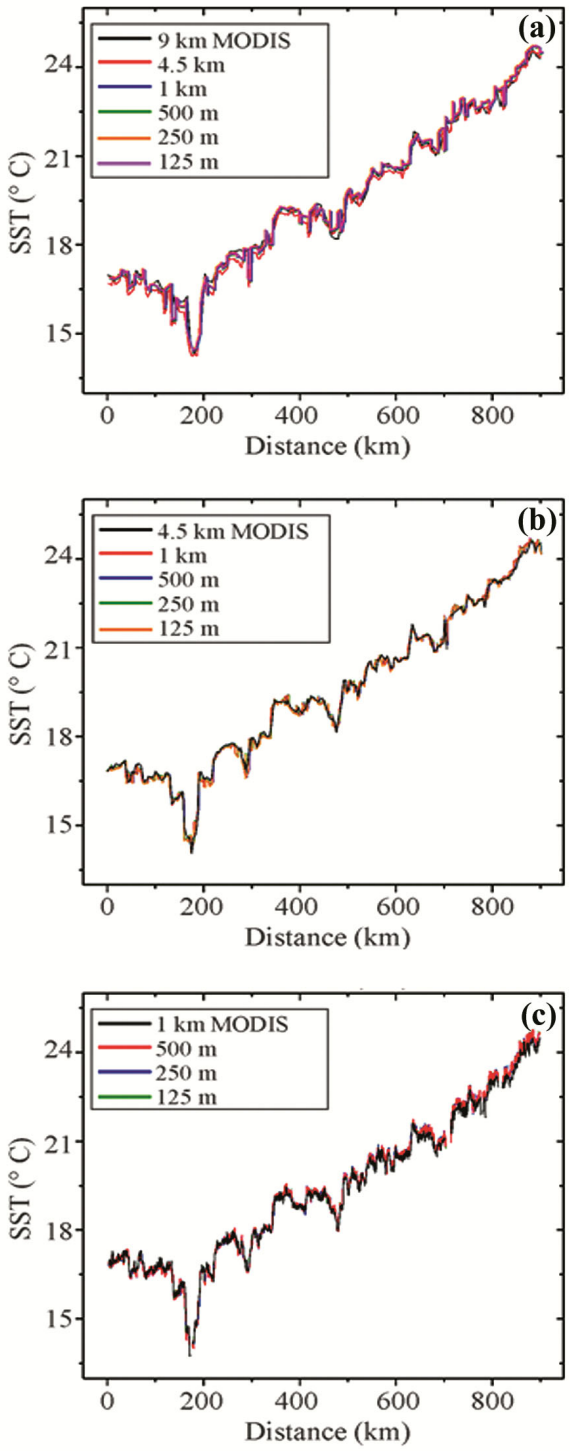

Fig. 4 — Downscaled Sea Surface Temperature (SST) along the 1000 km transect (T1) based on a sampling area extraction of 1-by-1 pixel size. (a) Downscaled 4.5 km, 1 km, 500 m, 250 m, and 125 m SST data based on the MODIS 9 km per pixel data, (b) Downscaled 1 km, 500 m, 250 m, and 125 m SST data based on the MODIS 4 km per pixel data, and (c) Downscaled 500 m, 250 m, and 125 m SST data based on the MODIS 1 km per pixel SST data

downscaled image derived from MODIS data at 9 km and 4.5 km, respectively. The findings of this study reveal that the linear associations exhibited a strong coefficient of determinations, regardless of the sampling area utilized for data extraction. Therefore, the utilization of the open-source algorithm is recommended for facilitating a feasible downscaling process.

The results presented in Figure 4 showcase the SST MODIS and downscaled SST values along the 1000 km transect in the GC. All the downscaled values exhibit a similar trend when compared to the original MODIS data. The profile measured at 9 km per pixel reveals a less detailed pattern than the downscaled data, and the Midriff Island area records the lowest SST values. Figure 5 illustrates examples between the three MODIS images and their respective downscaling in the Midriff Islands area, which recorded the highest SST variability in the entire CG. Results below the spatial resolution of 250 m per pixel have not been displayed as they are not distinguishable visually. The spatial pattern of the MODIS image at 1 km per pixel fits quite well, with the image downscaled to 1 km per pixel from the MODIS image at 9 km and 4.5 km. Hence, it was possible to match the SST spatial pattern with the open-source algorithm even up to a processing level of 125 m per pixel. Overall, the downscaled images provide more detail than the original MODIS data.

Discussion

This research employed an open-source algorithm to approximate SST by analyzing three distinct data sources from the same MODIS-Aqua sensor with varying spatial resolutions (9 km, 4.5 km, and 1 km). The limitations of utilizing a solitary data source from level 2 are acknowledged in the methodology section. However, these limitations should not affect the approach adopted as the open-source algorithm separately downscaled the three final datasets.

In cases where a strong SST gradient is present, such as in the GC[13], using an extraction method that integrates 1-by-1 and 3-by-3-pixel sampling areas can be beneficial. This study proposes a spatial downscaling approach that transfers data with lower spatial resolution into an SST matrix with finer spatial resolution without relying on commercial or black-box software. As a result, this work demonstrates the feasibility of the open-source algorithm to project SST data on a much larger scale without compromising the overall trend in the spatial

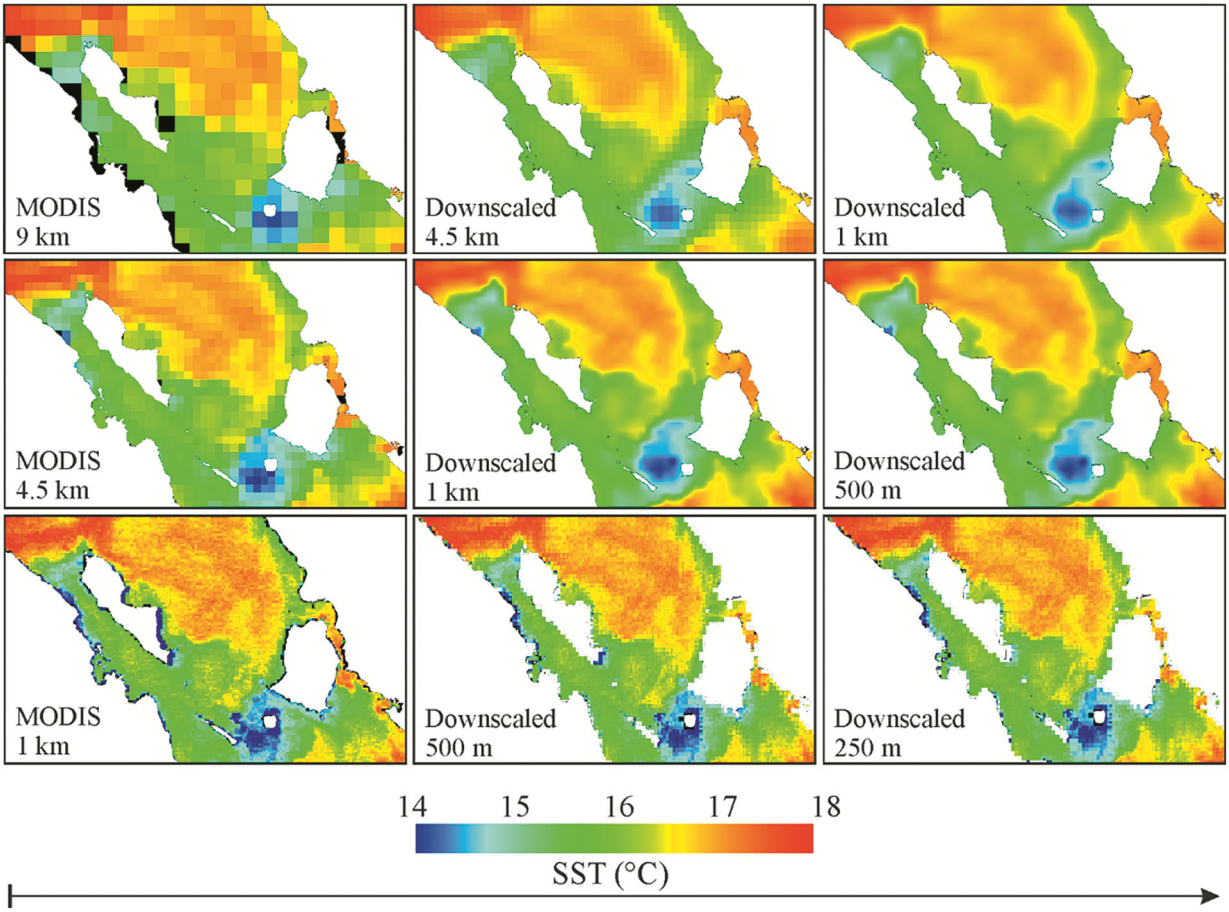

Fig. 5 — Spatial distribution of downscaled Sea Surface Temperature (SST) at the Midriff Islands area based on three data sources from the MODIS-Aqua (9 km, 4.5 km, and 1 km). From left to right, original MODIS data and their respective downscaled images

distribution pattern. It is noteworthy that any of the pixel extractions can be utilized when modeling the SST, as the results were found to be highly similar. Despite technological advancements, issues regarding achieving optimal computational performance exist. These challenges are comprehensively discussed in the following text.

Several techniques have been developed to downscale data but are often evaluated separately, without comparison[23]. As a result, few studies have been conducted to assess the accuracy of different spatial resolution data sets[17]. Downscaling techniques pose a significant challenge, as their effectiveness relies on the clear link between the nature of spatial variation and the sampling efficiency[15]. However, the results of the linear trend between the SST MODIS data at 4.5 km and 1 km and the data reduced to 4.5 km and 1 km, obtained from different initial spatial resolutions, showed minimal differences in the modeling of SST using different sampling areas (1-by-1 and 3-by-3-pixels). Additionally, as Xu[24] suggested, a visual comparison of the downscaled images, such as in Figure 5, indicates that the proposed approach successfully reproduces the SST spatial pattern.

The analysis reveals that the spatial resolution and sampling areas of the MODIS and downscaled data differ but exhibit similar patterns. The observed SST pattern along the longitudinal transect of the GC supports this. However, the accuracy estimation may be affected by data clustering, and the results may also be influenced by the selected downscale algorithm[17]. In the case of strong spatial gradients, such as the SST recorded in the CG, the coefficient of determination between measured and estimated values tends to increase regardless of the method used[15]. Furthermore, the spatial distribution of the data may also impact the performance of the spatial reduction method[17]. The open-source downscaling algorithm employed in this study produced positive outcomes in

this marginal sea, possibly due to the presence of SST gradients.

It is of utmost importance to consider the computational efficiency of downscaling techniques, especially in real-time applications[25]. Although all SST values replicated the spatial pattern of the original MODIS data, the downscaled images provided more intricate details, resulting in a notable increase in the time required to generate files, particularly for higher levels of detail (*e.g*., 500 m, 250 m, and 125 m from the 9 km MODIS image). The large data density of the extracted 3-by-3-pixel sampling area presented a significant challenge for downscaling SST, given that a much larger area was extracted per pixel. Although it was possible to achieve a similar spatial pattern among the images, it is essential to acknowledge the primary limitations of this study. For instance, the spatial accuracy of downscaling algorithms is affected by various factors, including the initial spatial resolution scale[26]. In this regard, the algorithm that utilizes a 1-by-1 pixel extraction considers the four neighboring pixels, irrespective of their original spatial resolution. Moreover, MODIS-Aqua images captured at different intervals (*e.g*., days, months, or years) may exhibit varying spectral characteristics, even in the absence of any scene changes, due to atmospheric fluctuations such as cloud cover, environmental temperature, and the position of the Sun over time[27]. Another important factor is data density, which influences the performance of spatial downscaling methods[17]. Without abundant, continuous data, the underlying assumption regarding the variation among neighboring pixels may differ, and the downscaling algorithm could increase the number of missing values[23]. However, this study could replicate the spatial pattern in the study area, even in coastal regions with no recorded values, as depicted in Figure 5.

Predicting coastal variables with remote sensing data is frequently a challenging task. Hence, the utilization of an open-source methodology for the estimation of SST can potentially be of great significance in providing swift and pertinent information regarding SST fluctuations along the short stretches of the coastline. For instance, coastal communities are increasingly at risk of extreme weather events such as flooding from tropical storms and hurricanes[28] and the impact of rising agricultural and river discharge flows, which can affect optical variables like chlorophyll-*a* concentration[2]. The approach adopted in this study can help evaluate river plume dynamics in regions where data with low spatial resolution is typically employed. Additionally, an open-source program affords us the necessary tools to analyze data without geographical limitations or the monetary need for licensed commercial software.

Conclusions

The study demonstrates that the open-source algorithm is feasible for reconstructing a single SST image across coastal and oceanic regions, such as the GC. Both quantitative and visual evaluations were performed to validate the results. It should be noted, however, that the downscaled SST matrix for each level depends on the original spatial resolution within each image. While the three original MODIS-Aqua data sets come from the same processing level, this potential limitation was irrelevant because the open-source algorithm processed the three matrices separately. More research is required to evaluate the findings at other representative sites with different oceanographic dynamics from those in the GC. Additionally, further work is needed to assess the performance of other downscaling algorithms based on the results obtained in this study.

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Conflict of Interest

No potential conflict of interest was reported by the authors.

Data Availability

The data that support the findings of this study are available from the corresponding author, [FFdS], upon reasonable request.

Author Contributions

RRS: Conceptualization, data curation, methodology, visualization, and writing–original draft preparation; LFAS: Conceptualization, data curation, software, and validation; and FFdS: Formal analysis, investigation, supervision, and writing–review & editing.

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