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Filling in Missing Sea-Surface Temperature Satellite Data Over The Eastern Mediterranean Sea Using the DINEOF Algorithm

Geoinformation Conference

Andreas Nikolaidis[1,2], Georgios C. Georgiou[2], Diofantos Hadjimitsis[1], Evangelos Akylas[1*]

1 Department of Civil Engineering and Geomatics, Cyprus University of Technology, 30 Arch bishop Kyprianou Str., 3036, Limassol, Cyprus

2 Oceanography Centre, University of Cyprus, PO BOX 20537, 1678, Nicosia, Cyprus

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Abstract: The Data Interpolating Empirical Orthogonal Functions method is a special technique based on Empirical Orthogonal Functions and developed to reconstruct missing data from satellite images, which is especially useful for filling in missing data from geophysical fields. Successful experiments in the Western Mediterranean encouraged extension of the application eastwards using a similar experimental implementation. The present study summarizes the experimental work done, the implementation of the method and its ability to reconstruct the sea-surface temperature fields over the Eastern Mediterranean basin, and specifically in the Levantine Sea. L3 type Satellite Sea-surface Temperature data has been used and reprocessed in order to recover missing information from cloudy images. Data reconstruction with this method proved to be extremely effective, even when using a relatively small number of time steps, and markedly accelerated the procedure. A detailed comparison with the two oceanographic models proves the accuracy of the method and the validity of the reconstructed fields.

Keywords: Remote Sensing • sea-surface temperature • DINEOF • data reconstruction • Levantine Sea

1. Introduction

Let us consider a basin filled with water whose surface is oscillating. To describe this surface wave we should note the position of every water particle at every moment, which rapidly generates a huge amount of data. During the last few decades there has been considerable effort put into finding simple (usually referred to as 'empirical') functions, which satisfactorily describes such a system. The most common approach is to use a spatial function that gives the form of the wave at a given moment and a temporal function which characterizes the variation of the wave over time. Determining these functions then avoids excessive data accumulation. In geophysics, a well-known and widely used method (introduced by Lorentz in the 50's) [1], is the geographically-weighted Principal Component Analysis (PCA), which is normally referred to as empirical orthogonal functions (EOFs). Specifically, PCA is defined as an orthogonal linear transformation that maps the data to a new coordinate system such that the greatest variance by any projection of the data comes to lie on the first coordinate (called the

*E-mail: evangelos.akylas@cut.ac.cy

first principal component), the second greatest variance on the second coordinate, and so on. EOFs can present different physical meanings, like coherent spatial patterns with maximum variance, modes of energy, or even just convenient mathematical abstractions, depending on the nature of the problem. Backers and Rixen [2] demonstrated an innovative EOF method that does not need any prior knowledge of the correlation function or correlation length from the data. Due to the iterative nature of the algorithm, any inhomogeneity or non-isotropic behavior is automatically taken into account, generating an interpolation effect, hence the name Data Interpolating Empirical Orthogonal Functions (DINEOF). An adaptation of handling large data sets (typical of satellite imagery) can be found in [3].

Filling in the gaps generated by the existence of clouds, rain, or simply due to incomplete track coverage is one of the most common problems faced while processing satellite data. Many methods have been tested over the years to solve this problem, with different results regarding the field of application and the expertise of the scientists involved. Notable examples are the Data-Interpolating Variational Analysis (DIVA) that allows the spatial interpolation of data (analysis) in an optimal way, and the optimal interpolation method. However, the DINEOF method is simply faster.

Optimal Interpolation (OI) is the classic and most well-known method. The main problem is the length of calculation time. For a typical ensemble of data, DINEOF is an innovative method, and 30 times faster than OI. This increase in speed is a direct consequence of the different statistical methodology used between the two different approaches. In particular, DINEOF constitutes a procedure that fills gaps by iteratively decomposing the data field via Singular Value Decomposition (SVD) until a best solution is found, as compared to a subset of reference values (non-gaps). This is done by progressively including more EOFs in the reconstruction of the missing locations until the minimization of error converges.

In this paper, we apply the DINEOF method in order to reconstruct a full satellite-derived sea surface temperature (SST) field, for the Eastern Mediterranean, Levantine sea and Cyprus coasts. SST is a physical parameter commonly used in most oceanographic and meteorological applications [4] and among others is a principal factor for relevant arithmetic model calibration, assimilation and initialization [5–7]. DINEOF is applied for the first time over the specific area of the Eastern Mediterranean Sea, a step which is crucial, both for the research as for the operational implementation of the method. The structure of this work is as follows. In Section 2 a description of the DINEOF method and of the corresponding algorithm is given. Section 3 describes the application of the method used in the Eastern Mediterranean Sea. Finally, in Section 4 the results of the implementation are analyzed and discussed.

2. Description

By using the EOF method, one is able to identify a set of orthogonal spatial modes, such that, when ordered, each successive eigenvector explains the maximum amount possible of the remaining variance in the data. Each eigenvector pattern is associated with a series of time coefficients that describe the time evolution of the particular spatial mode. The eigenvector patterns that account for a large fraction of the variance are, in general, considered to be physically meaningful and connected to important 'centers of action'.

The EOFs can be regarded as eigenvectors, which are aligned so that the leading EOFs describe the spatially coherent pattern that maximizes its variance [8]. EOFs are often used as a functional basis (a new set of axes or reference frame), providing a convenient method for studying the spatial and temporal variability of long time series data, over large areas. The method splits the temporal variance of the data into orthogonal spatial patterns called empirical eigenvectors. The EOF analysis may be thought of as being analogous to data reconstruction based on Fourier transforms (FT), in the sense that they both produce series (vectors) which form an orthogonal basis. In the following, we briefly summarize the mathematical principles of the algorithm.

2.1. 2.1 PCA-SVD-EOF

The Principal Component Analysis tries to explore the question *'can our data set be expressed better in one other basis which is a linear combination of our current basis?'* The answer to the above identifies the existence of linearity, noise, and correlations in the data. In order to explain the way this method works, one may assume two data sets $A = \{a_1, a_2, .., a_n\}$ and $B = \{b_1, b_2, .., b_n\}$, $n \geq 1$. Their variances will be $\sigma_A^2 = \frac{1}{N}\sum_i^N (a_i - \mu_A)^2$ and $\sigma_B^2 = \frac{1}{N}\sum_i^N (b_i - \mu_B)^2$ respectively, where $\mu_A = \frac{1}{N}\sum_i^N a_i$ and $\mu_B = \frac{1}{N}\sum_i^N b_i$ are the mean values of the data sets. Hence the covariance between A and B sets will be $\sigma_{AB}^2 = \frac{1}{N}\sum_i^N (a_i - \mu_A)(b_i - \mu_B)$. The covariance matrix is a measure of the degree of linearity between two variables. In other words, it is a measure of the proportion of the

variance of a set that can be explained through a linear relation from the respective variance to that of the other one. A large positive value indicates positively correlated data. On the other hand a large negative value denotes negatively correlated data. The absolute magnitude of the covariance measures the degree of redundancy.
If σ_{AB} is zero, then sets A and B are uncorrelated. The equality $\sigma_{AB}^2 = \sigma_A^2 = \sigma_B^2$ holds if and only if, $A = B$. All the methods applied here yield a finite number of modes that represent the covariance matrix of the data. Its rows and columns indicate the covariance (or correlation) between the time-series at a given station or grid-point of one field and the time-series at all stations or grid-points of the other field. Singular Value Decomposition (SVD) analysis offers the same types of normalizing and scaling options as EOF analysis (i.e. it can be based on either the covariance matrix or the correlation matrix). Each mode in the analysis is identified by an eigenvalue (a positive distinct number which defines its rank and relative importance in the hierarchy of modes), an eigenvector or EOF (a linear combination of the input variables in the domain of the structure), and a principal component (PC) which documents the amplitude and polarity of that structure in the sampling domain. It should be noted that a common measurement of the feasibility of the PCA application is the Signal-To-Noise (SNR) ratio. SNR is defined as $SNR = \sigma_{signal}^2/\sigma_{noise}^2$ which in practice is the ratio of the variances. A high SNR ($\gg 1$) indicates a high precision measurement, while a low SNR indicates very noisy data [9]. If PCA is made by using SVD then the output consists of the eigenvalues plus two rectangular matrices. The context of the analysis will determine which one should be labeled the Empirical Orthogonal Function (EOF) matrix and which one the Principal Components (PC) matrix.

2.2. The algorithm

Recalling the description given by Alvera-Azcarate *et al.* [10], we consider an $M \times N$ matrix X, M and N being the spatial and temporal sizes, respectively. Anomalies are computed and the missing data are normalized to the mean (i.e. to a zero anomaly). Initially the most dominant EOF mode of this matrix is obtained, and the missing data are calculated by means of

$$X_{m,n} = USV^T \tag{1}$$

where $m = 1, \ldots, M$ and $n = 1, \ldots, N$. U is an $m \times r$ matrix representing the spatial EOF nodes, V^T is an $n \times r$ matrix containing the temporal modes, and S is an $r \times r$ matrix containing singular values. The value $r \leq \min(m, n)$ is the rank of the X matrix. For the reconstruction of X, only the most significant spatial and temporal EOF is used. The new estimation of X for the missing data is reintroduced into the data matrix, and the EOF mode calculation is repeated. This process is continued in a successive fashion until the convergence of the missing values, and consequently the EOF modes calculated, are increased to two, then to three, etc. The EOF mode calculation is succeeded using a Lanczos solver provided by the ARPACK free software. A major improvement on the latest DINEOF version, is the ability of outlier detection, provided by the ratio between the analysis residuals and their expected standard deviation,

$$O_i = \frac{X_i^a - X_i^o}{\Delta_i} \tag{2}$$

For non-missing, original values X_i^o are given, where $i = 1, \ldots, m$ is the spatial index, X_i^a is the new value, as created by DINEOF, and Δ_i is the expected misfit, calculated by

$$\Delta_i = \sqrt{\mu_{eff}^2 - \sum E_{i,k}^2} \tag{3}$$

In the above, $i = 1, \ldots, N$ is the number of EOFs used from the algorithm for the reconstruction, while $k = 1, \ldots, N$ are all used modes. Parameter u_{eff}^2 is an estimation of the average noise of the initial field, obtained as a cross-validation error. The expected error $E_{i,k}$ of each $i-$position is calculated by

$$E = L_p S_c \quad \text{with correlation matrix} \quad C = S_c S_c^T \tag{4}$$

where L_p is constructed by $m \times N$ columns of the spatial EOFs multiplied by the corresponding singular values, and Sc is the $N \times N$ Cholesky factorization of the C correlation matrix. More details on the mathematical procedure can be found in [11]. In Figure 1, the outline of the implementation of the DINEOF algorithm is presented.
The optimal number of EOFs needed to calculate the missing data is determined by cross-validation: a small percentage of valid data (typically 1% of the total data) is initially set apart and flagged as missing. Once convergence is reached for a given number of EOF modes, a root mean square error is calculated between the newly obtained estimate and the initial dataset. The number of modes that minimizes this error is considered as optimal. It is notable that not all modes need to be calculated, as one can observe that when the error increases steadily for 3 consecutive modes, a minimum

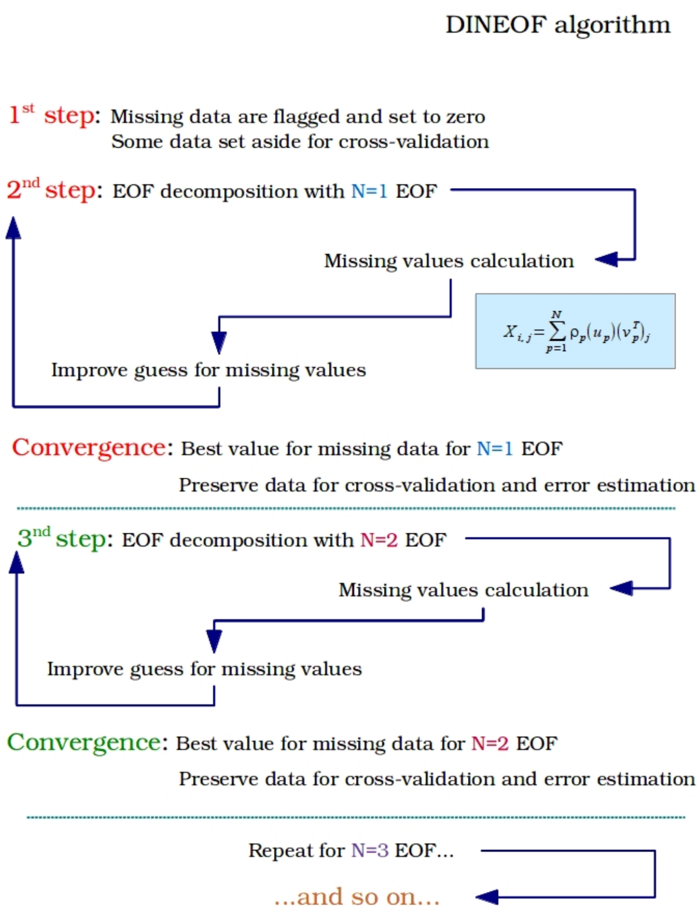


Figure 1. DINEOF algorithm iterative scheme (based on [11].

has been reached [11]. The optimal number of EOF modes retained is calculated by cross-validation (i.e., a few valid data are set aside and the error of the reconstruction is assessed by comparing the reconstructed data to these cross-validation data). For an extended description of DINEOF, and recent developments, the reader is referred to Beckers and Rixen [2], Alvera-Azcárate *et al.* [3, 12] and Beckers *et al.* [13].

3. Application

The DINEOF algorithm has been successfully implemented over the Western Mediterranean in a continuous basis by GeoHydrodynamics and Environment Research, a research group at the University of Liège, where they produce daily, cloud-free SST images for that area [11]. The scope of the present work is the extension of the DINEOF algorithm application over the Eastern Mediterranean Sea. Until now, there has been no known procedure that systematically recovers missing data from satellite images for the full area covering the Levantine Sea and Cyprus coasts. However, cloud-generated noise is frequent, especially during winter and spring, resulting in incomplete information which is important for lots of applications. The present application aims at recovering missing SST data from sparsely covered satellite images. The data refer to SSTs measured twice a day at 10:00 am and 20:00 pm GMT and cover the area from southern Italy to the Middle East (Figure 2) with atmospheric corrections. The data are collected collaboratively by Meteo-France and the Norwegian Meteorological service (DNMI) just 2 hours after the last satellite data acquisition. The same type of data, L3 from

MERIS satellite products, is used for the aforementioned Western Mediterranean project. In this case study, the radiometry satellite data covers a total of 400×500 cells on a geographical grid with a spatial resolution of 2220 m.

A typical example of initially incomplete data is shown in Figure 2 (left), for the 11th of January 2013. In order to recover the missing information, DINEOF code version 3.0, provided by GHER website, has been used. Although, in the case of the Western Mediterranean, the application is based on a long-term sample collection, in this work we have chosen to perform the experiment only in a 4 day period from the 9th to the 12th January 2013 (Figure 3). It is suggested that the reduction of the sample size markedly accelerates the procedure without seriously affecting the accuracy. The effectiveness of the application can be more clearly shown if one separates a rather "empty" input image, and provides the corresponding result in Figure 2 (right). It is suggested that the longer the available time-series, the better the results will be in relation to the area covered [10]. However, a question regarding the quality and the validity of the generated results and their dependence on the sampling size still remains. In our opinion, a reduction in the sampling size in terms of its dependence on the historic data offers a less-biased reproduction of local rapid changes. Nevertheless, "first-guess" information exists, where no information was available. Or at least, there is strong evidence of the dominant factors around the area of interest. EOFs were performed on the 'cloudy' data received from the satellite dataset. Results from the current application on a 12-hour basis from the 9th to the 12th January 2013 are given in Figure 3. It should be noted that heavy clouds between the 11th and 12th of January could have easily led to extreme values and corruptions in the SST field. The accuracy obtained with the DINEOF application, as it will be shown, is mainly due to two reasons: the filtering of spikes in the temporal EOFs, and the standard number of EOFs that were retained in the Eastern Mediterranean Sea. For the current application, the same model set-up parameters have been used for all cases. After several different runs and continuous testing, it has been concluded that calculations with five (5) EOF modes, using the application's default threshold (10^{-8}), without modifying the existing data (the original satellite images) and without normalization of the results, rendered the most satisfactory results. Keeping the first five EOFs in the area under consideration, proved the best choice, allowing for reconstruction and capturing of even small scale variability. It is known that the higher order EOFs do not only contain small-scale information, but also noise.Forcing DINEOF to retain a higher number of EOFs than was calculated with the cross-validation method should be done with caution, as this might degrade the overall quality of the reconstruction.

4. Validation of the results and discussion

In order to estimate and test the successful implementation of the application presented here, a comparison of the recovered results against the outputs of oceanographic models that provide regional now-casting real time information is performed. Two of the most important and relevant models, are:

1. the CYCOFOS [14], the Cyprus Operational Oceanographic System, providing high-resolution, detailed and accurate data from around Cyprus and in the Levantine sea, and

2. the U.S. Navy Coastal Oceanographic Model [15], which covers a wider area, at a lower resolution.

Both models are used in an operational basis by the Cyprus Government, the US Navy and Research Institutes around the world (including MyOcean [16], SeaDataNet [17] and numerous scientific organizations in the European Union, and others, including GOOS, IOC/UNESCO).They have been deeply studied and tested. In Figure 4, we outline the testing procedure; (a) the initially cloudy image is regenerated with DINEOF; (b) as explained, the respective model's output for the same time is selected; (c) the differences between (b) and (c) at all points are computed; and (d) the same procedure is followed for each time-step for both models.
Firstly, comparison is made with the less detailed model US NCOM, as shown in Figure 5. The deviation of the model from the recovered SST values is illustrated. For all the time-steps, it is evident that the recovered data partially overestimate the SSTs compared to the model. Although, over most of the studied area, the differences remained relatively small (less than 1°C); near the Eastern Mediterranean coastal area the difference peaks at around 4°C. This difference could be intuitively attributed to the fact that the specific area lacks original SST information as shown in Figure 3. In other words, this difference could be due to DINEOF's inaccuracies. However, this is not true. The US NCOM model covers the area in a lower resolution resulting in less accurate results. In fact, Figure 6, which focuses on the vicinity of Cyprus through the CYCOFOS operational model, shows a high level of agreement between the model results and the DINEOF predictions. As mentioned, CYCOFOS is a

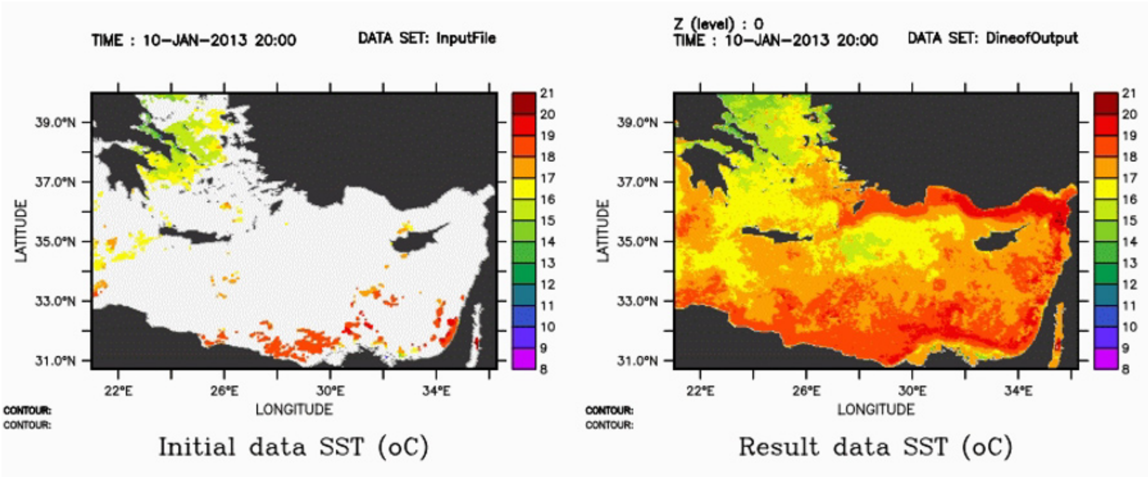
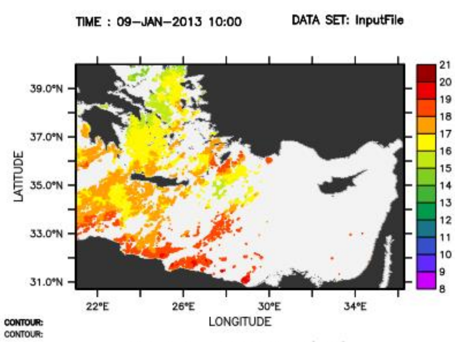


Figure 2. A typical example of a cloud-covered area during the data collection (left), and its recovered information (right) over the area of application.

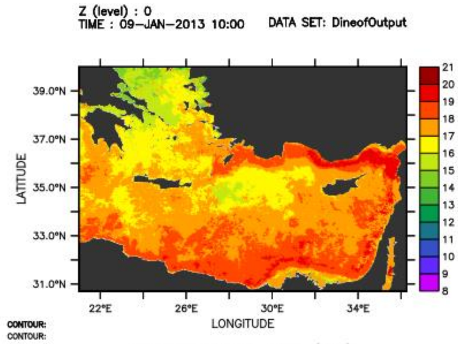
source of very accurate data, providing high-resolution data for the Cyprus coasts and Levantine Sea. The observed agreement, with absolute differences of less than 1°C, is further verified by respective in-situ measurements from the Paphos tide-gauge station (data available from CYCOFOS web site), revealing the same behavior.

In Figure 7, the detailed SST fields from the CYCOFOS model and the respective ones from the application of the DINEOF procedure are illustrated. This illustration is crucial in order to test the basic pattern and the main physical characteristics of the recovered SST fields. As noted, a general clear difference of the order of one degree Celsius for all the period is observed between the two cases, with the DINEOF estimating lower SST values. This difference is considered acceptable, especially since the comparison is done against modelled data. Furthermore, it is evident that the models almost certainly use a thicker upper layer than the one the satellite sees, depending on the sigma layer construction used. In particular, in the case of the two models presented, this layer is almost 2 m thick. As a result, at the specific satellite observation times, the temperature at the sea surface is expected to be slightly higher than the average temperature of the above layer. This could possibly explain the systematic divergence of the order of −1°C between the recovered SST and the modelled pattern.

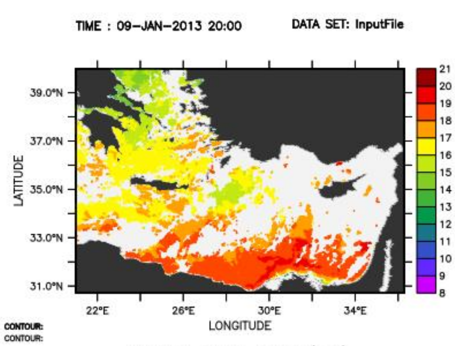
In fact, observing the DINEOF results in detail, one may identify some remarkable features. The high temperatures that appear near the Asia Minor coast are a good indicator of the consistency of the reconstructed values real data, with respect to historical climatologic SST values from the specific area. Furthermore, the profound concentrations of colder water that appear in the North West area, in agreement with the known cold water formations near the Ierapetra gyro, are a further indication of success. Finally, the existence of remarkably lower temperature patterns near the Palestinian coasts could have been the natural result of the impact of the Cyprus gygo [18]. The above comments show that all the information obtained by the reprocessed satellite data concerning SST constitutes a good, acceptable representation of the known conditions and of the impact of the main physical mechanisms that influence the studied area. The resulting DINEOF representation could even prove more detailed and accurate results compared to the CYCOFOS model. For instance the DINEOF application shows lower SST values (around 16°C) along the western Cyprus coast compared to the 17-18°C estimation of the model. The in situ measurements from Paphos tide-gauge station for the same period vary between 15°C and 16°C, showing a better agreement with the DINEOF results. The overall success suggests the existence of a strong basis available for further testing and application, including more sophisticated procedures, in the direction of successfully implementing a continuous recovery of SST data from satellite images over the Eastern Mediterranean. It is expected that in the future such results could serve as input for assimilation processes and model calibrations.



Initial data SST (oC)



Result data SST (oC)



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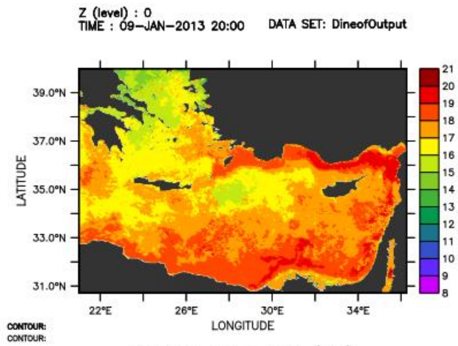
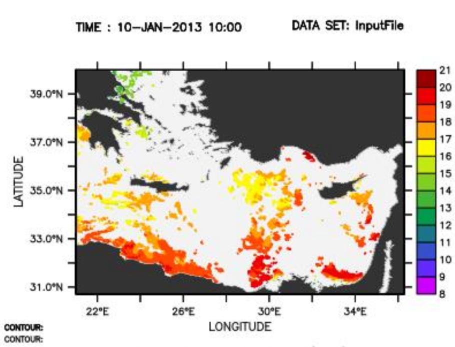
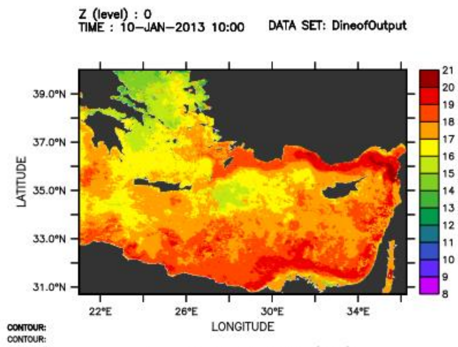


Result data SST (oC)



Initial data SST (oC)



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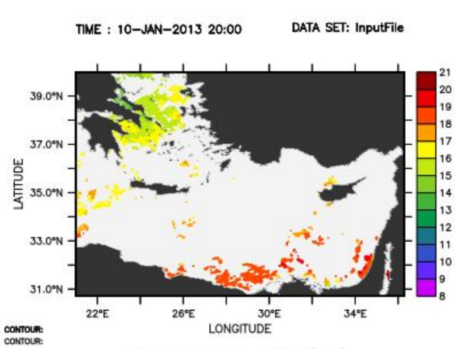
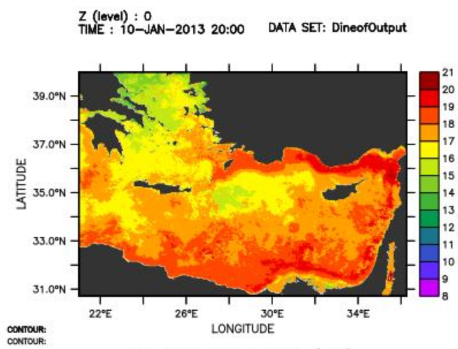


Initial data SST (oC)



Result data SST (oC)

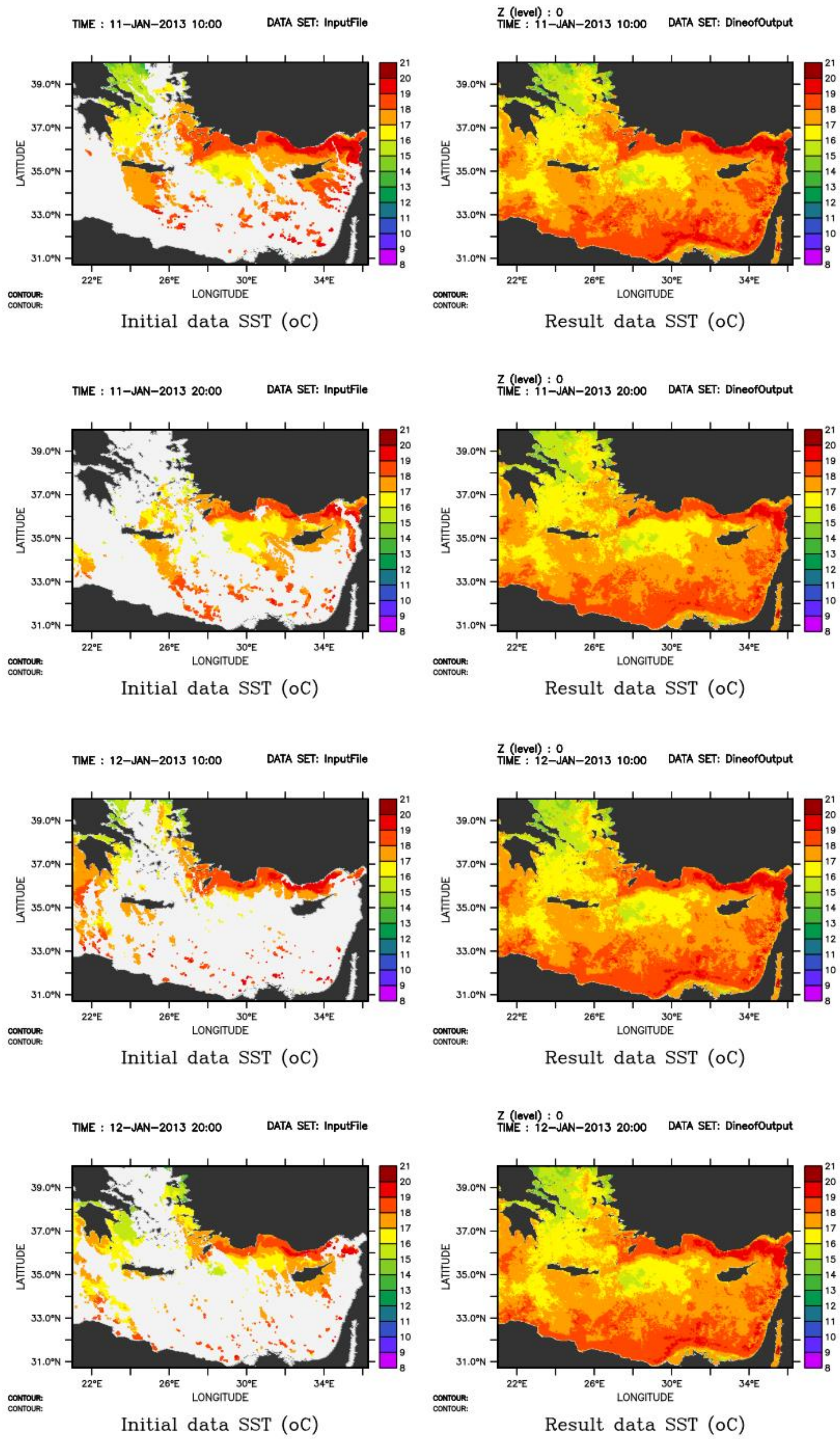


Figure 3. Original and reconstructed SST data for the Eastern Mediterranean for the period 9 - 12 /1/2013.

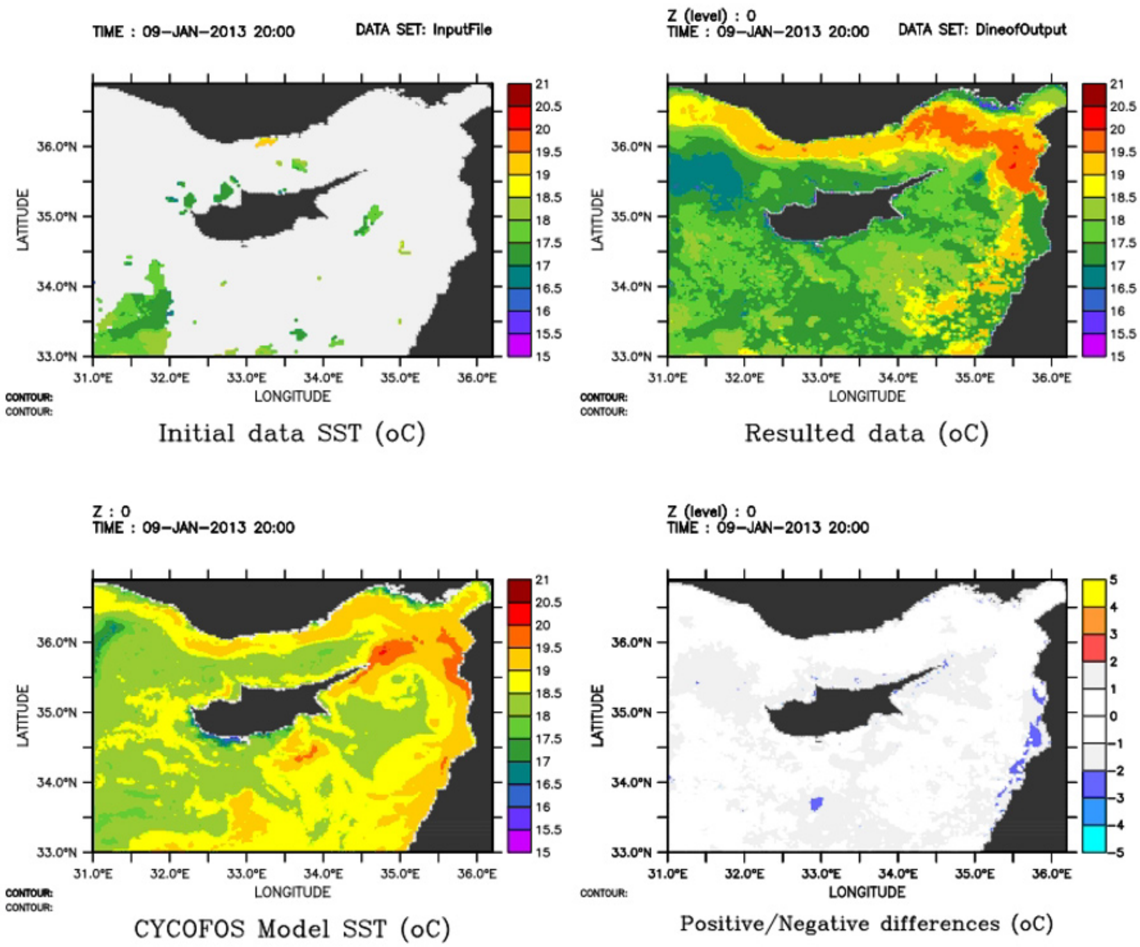


Figure 4. Outline of the validation procedure for an arbitrary time-step for Eastern Mediterranean SST data.

5. Conclusions

The Data Interpolating Empirical Orthogonal Functions method is a special technique used for the reconstruction of missing data from satellite images. It is an innovative method, especially useful for filling in missing data from geophysical fields. SST is a physical parameter commonly used in most oceanographic and meteorological applications and among others is a principal factor for relevant arithmetic model calibration, assimilation and initialization. Previous work reported successful implementation of DINEOF in recovering missing SST data over the Western Mediterranean area. The DINEOF method has been applied in order to recover a full satellite-derived sea surface temperature field, for the first time over the Eastern Mediterranean, Levantine sea and Cyprus coasts. This is a crucial step for the operational implementation of the method. The results are really impressive, recovering data from very cloudy images with remarkable efficiency. The comparison against widely used highly accurate simulations revealed close agreement with differences not exceeding 1°C. The same quantitative agreement also holds true against in-situ measurements from the Paphos tide-gauge station. It should be stressed that this agreement is in favor of the DINEOF reconstructed results compared to the results produced by the detailed CYCOFOS model. The overall success suggests the existence of a strong basis available

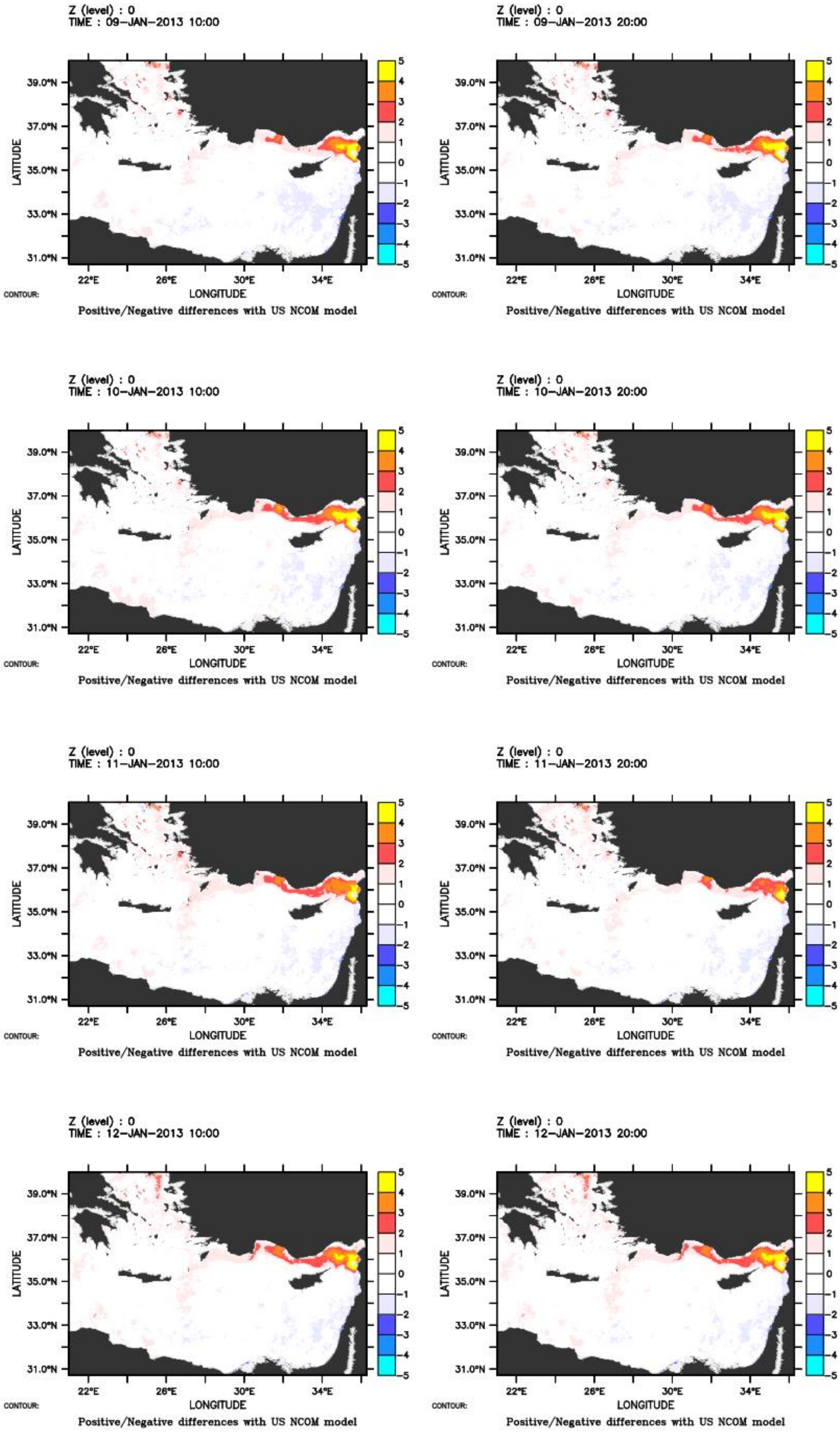


Figure 5. Computed SST differences between the present DINEOF application and the US NCOM model data.

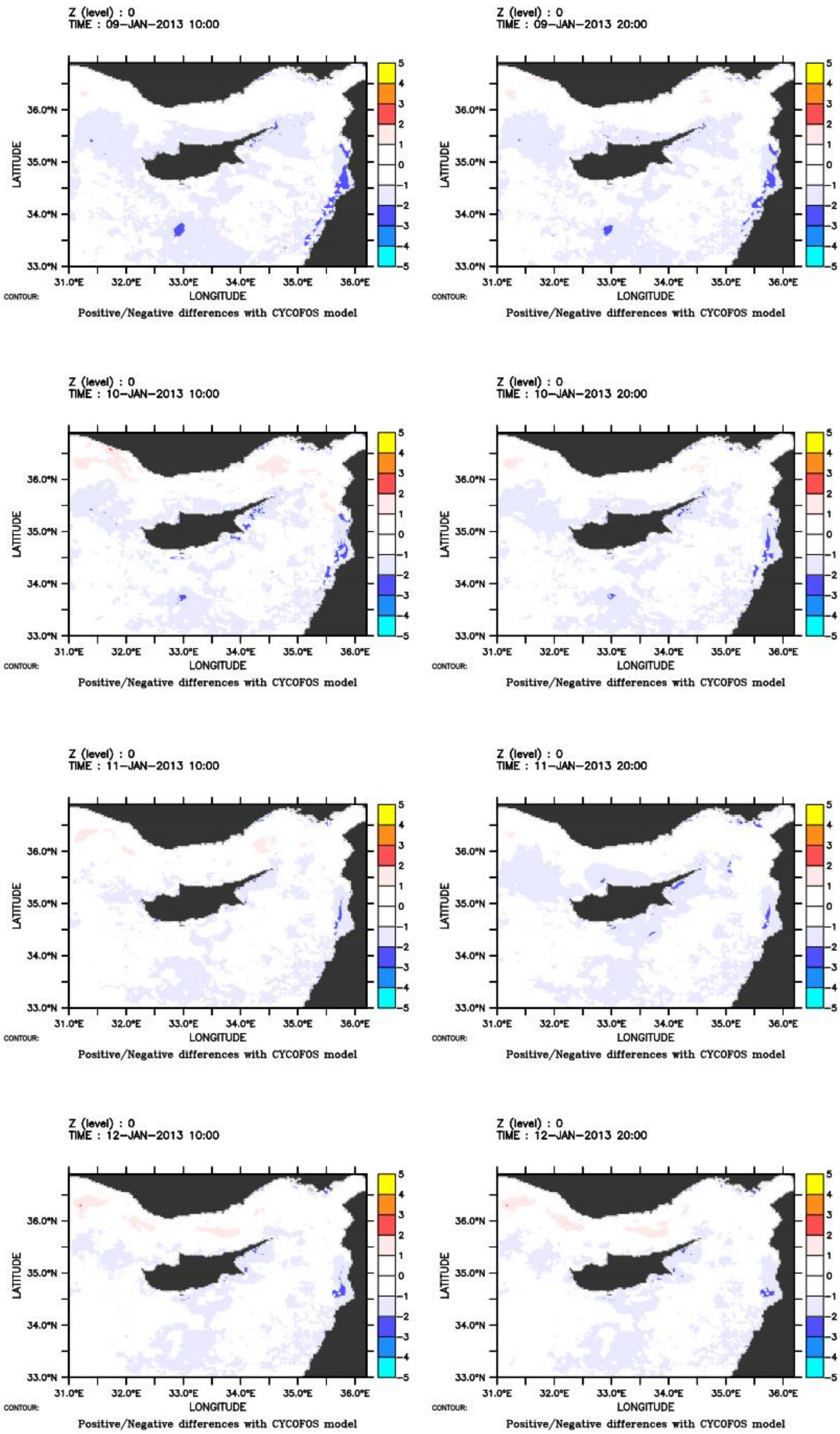
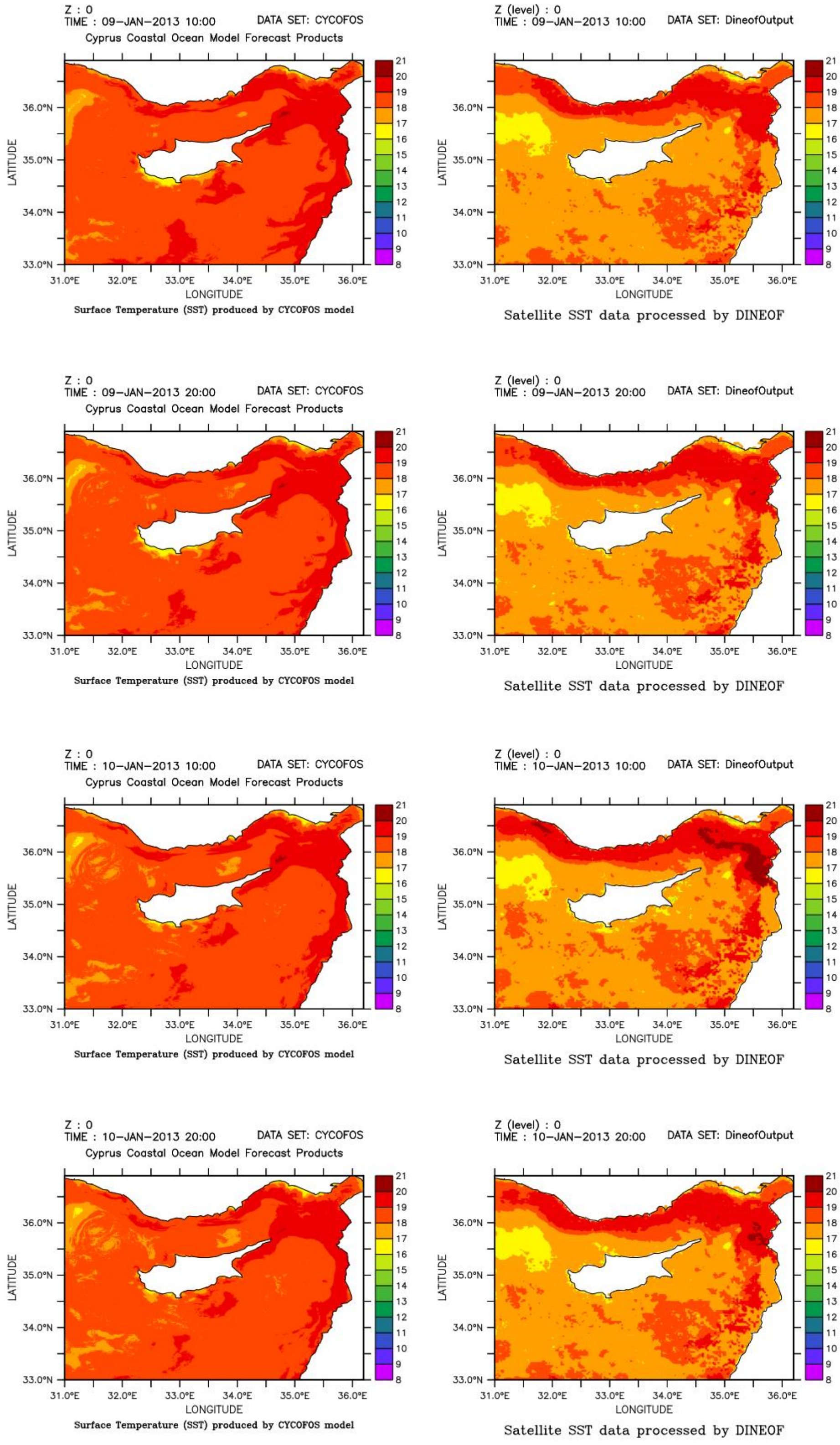


Figure 6. Computed SST differences between the present DINEOF application and the CYCOFOS model data.


Z : 0
TIME : 09–JAN–2013 10:00
DATA SET: CYCOFOS
Cyprus Coastal Ocean Model Forecast Products
Surface Temperature (SST) produced by CYCOFOS model
Z (level) : 0
TIME : 09–JAN–2013 10:00
DATA SET: DineofOutput
Satellite SST data processed by DINEOF
Z : 0
TIME : 09–JAN–2013 20:00
DATA SET: CYCOFOS
Cyprus Coastal Ocean Model Forecast Products
Surface Temperature (SST) produced by CYCOFOS model
Z (level) : 0
TIME : 09–JAN–2013 20:00
DATA SET: DineofOutput
Satellite SST data processed by DINEOF
Z : 0
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Cyprus Coastal Ocean Model Forecast Products
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Z (level) : 0
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Satellite SST data processed by DINEOF
Z : 0
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DATA SET: CYCOFOS
Cyprus Coastal Ocean Model Forecast Products
Surface Temperature (SST) produced by CYCOFOS model
Z (level) : 0
TIME : 10–JAN–2013 20:00
DATA SET: DineofOutput
Satellite SST data processed by DINEOF
LATITUDE
36.0°N
35.0°N
34.0°N
33.0°N
LONGITUDE
31.0°E
32.0°E
33.0°E
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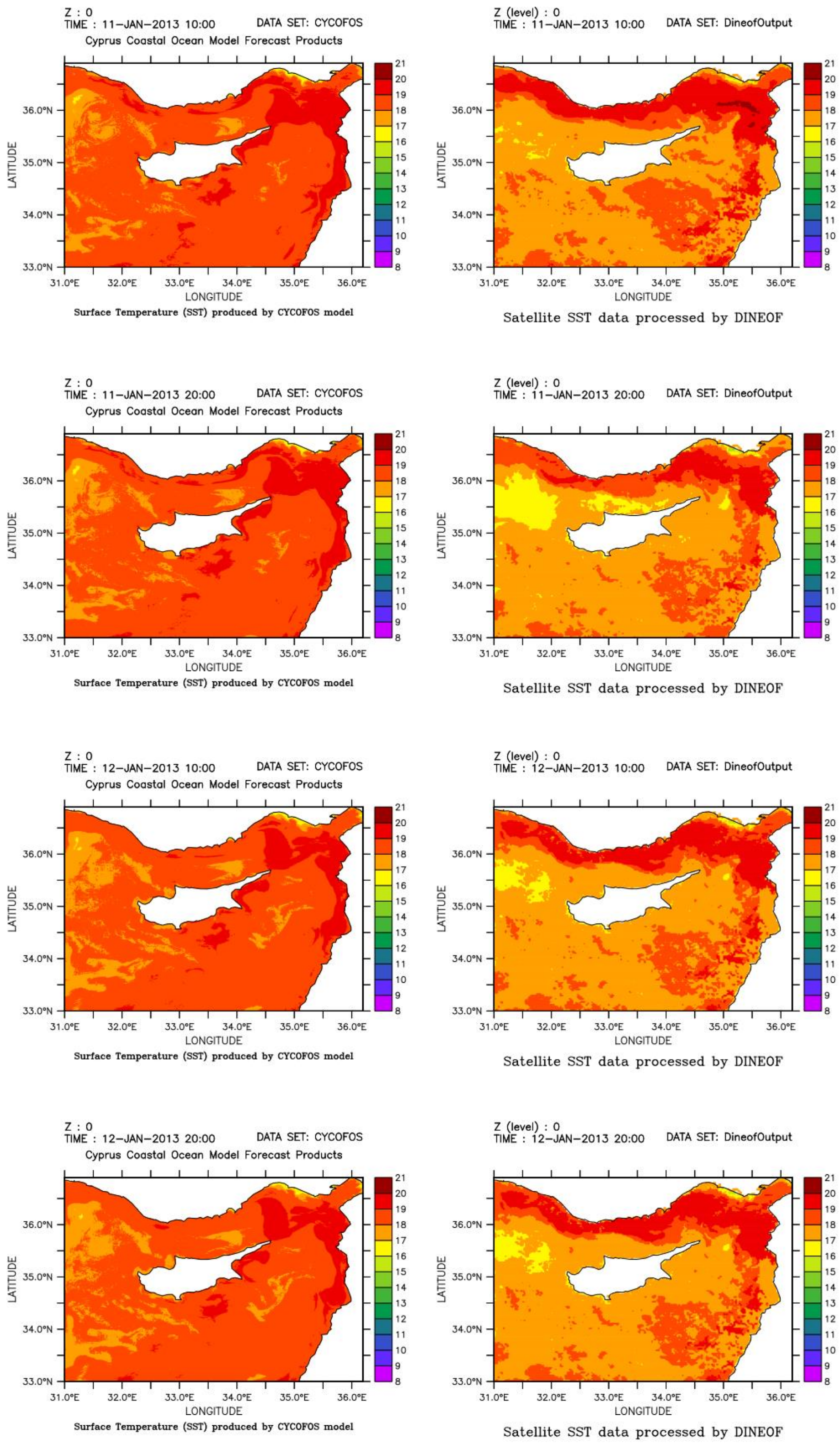

Figure 7. Comparison of SST estimates by DINEOF processed satellite data and the CYCOFOS model results.

for further testing and application. The method, provides reliable information, even better than that estimated by physical models, and may serve as a continuously updated basis for improved data for physical model assimilation (oceanography and meteorological-atmospheric models) and for better model tuning during operation.

Besides the impressive outcome of the DINEOF algorithm recovering SST data, the application of the method is not restricted to satellite processing. Using DINEOF, [19] studied the relationships between surface winds, the SSTs and Chl-a variations in the South Atlantic during 2003. Sirjacobs *et al.* [20] effectively applied the DINEOF method to study the case of suspended matter in the North Sea. In addition, similarly to the present application, daily DINEOF cloud-free SSTs for the Western Mediterranean Sea and for the Canary-Madeira region are produced on an operational basis [21]. There also exists a simplified R-project package, specially designed for adoption into this statistical environment. Due to the simplicity of the method, and the high-quality results, it is easy to leading to better quality reconstructed results from sparse datasets. This could be achieved by using a special dedicated geo-statistical tool, like those included in a GIS, for further optimization of results. This is a main topic for future research.

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