Neural Synthetic Profiles from Remote Sensing and Observations (NeSPReSO): Reconstructing temperature and salinity fields in the Gulf of Mexico.

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Introduction

Numerical models of the Gulf of Mexico (GoM) are crucial for various sectors due to the significant impact of GoM Loop Current (LC) and Loop Current Eddies (LCE) on climate, fisheries, and hurricane prediction. While the LC facilitates heat transport and features strong currents, LCEs influence oil and gas operations and hurricane intensity. Despite advancements in modeling, the sparseness of in situ data limits accurate subsurface circulation forecast.

Satellite data aids surface-level modeling, but subsurface measurements, mainly from the Argo program and specialized floats like LC-floats and UGOS 3, are very sparse, affecting mesoscale circulation accuracy. Techniques like Gravest Empirical Modes (GEM) and Improved Synthetic Ocean Profile (ISOP) generate synthetic profiles to enhance models, yet issues such as computational demand, accuracy and linear limitations persist.

Machine learning (ML) has shown promise in the GoM for various applications, from predicting LCE events to estimating carbon dioxide variations. Specifically, convolutional neural networks (CNNs) using satellite data have been explored for three-dimensional salinity field reconstruction. We introduce NeSPReSO, a method leveraging ML to estimate subsurface profiles using satellite and Argo data, aiming to improve computational efficiency and model accuracy. We investigate NeSPReSO's effectiveness against traditional methods and its potential for operational model integration.

Data

This study utilizes a mix of in situ and satellite data, the Argo float dataset is composed of 4,145 T and S profiles from 2015-2022 in the GoM, providing measurements up to 1,800 meters. For satellite data, we use Absolute Dynamic Topography (ADT) from CMEMS, Sea Surface Temperature (SST) from OISST, and Sea Surface Salinity (SSS) from SMAP as input parameters for our model. These datasets, with daily resolutions and fine spatial granularity, were interpolated to match the Argo and glider data points. ADT adjustments (subtracted the mean in the GoM) were made to account for seasonal upper ocean thermal expansion and contraction. Glider data from four missions targeting mesoscale structures are also used to validate our model. These have a vertical resolution of 5m. Figure 1 shows the T-S diagram of the dataset and highlights the core of the main water masses in the region: Gulf Common water (GCW), North Atlantic Subtropical Underwater (NASUW), and Sub-Antarctic Intermediate water (SAAIW), and the location of the profiles. Principal Component Analysis (PCA) is performed on this dataset, and the Principal Component Scores (PCS) are used to train and validate our model.

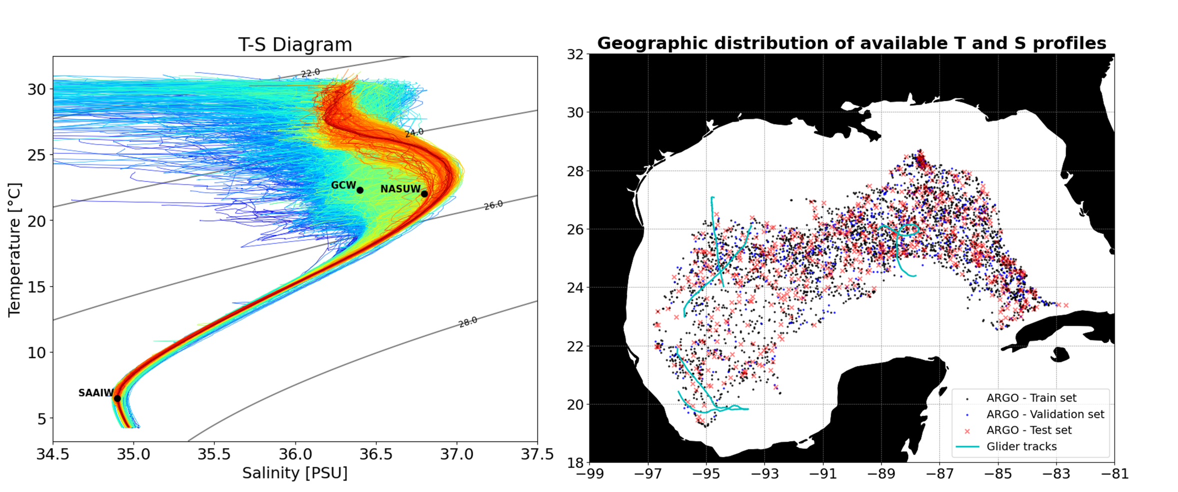

Figure 1: Temperature-Salinity diagram (left) and Spatial distribution (right) of the Argo profiles used in this study. The core of the Gulf Common water (GCW), North Atlantic Subtropical Underwater (NASUW) and Sub-Antarctic Intermediate water (SAAIW) are marked for reference.

PCA

We use PCA dimensionality reduction. We computing the covariance matrix $\mathbf{S}$ from the centered data matrix $\mathbf{Y}$:

$$\mathbf{S} = \frac{1}{n}\mathbf{Y}^T\mathbf{Y}$$

Then solve for eigenvectors $\mathbf{V}$ and eigenvalues $\mathbf{D}$ in $\mathbf{SV} = \mathbf{DV}$. Projecting $\mathbf{Y}$ onto $\mathbf{V}$ yields the PCS:

$$\mathbf{Z} = \mathbf{YV} \tag{1}$$

We can reconstruct the approximated data with $\hat{\mathbf{Y}} = \mathbf{ZV}^T$. To reduce dimensionality, $\mathbf{V}$ and $\mathbf{Z}$ can be truncated, keeping only the indices corresponding to the largest eigenvalues.

We apply PCA to T and S datasets separately, reducing from 1801 to 15 variables for each, and retaining significant variance (99.8% for T and 99.4% for S). The neural network is trained to predict these 30 PCS for each profile in the Argo dataset, allowing for efficient training and reconstruction.

Acknowledgments

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NN Architecture

Let $X \subset R^{d_X}$ be our input space (possible surface measurements) and $Y \subset R^{d_Y}$ the output space (possible vertical profiles). Our ultimate goal is to find a mapping operator $\Phi : X \to Y$ that for all measurement vectors $x \in X$, there exists a corresponding T and S profile $y \in Y$ such that $y = \Phi(x)$.

Suppose the output space Y can be encoded into a space $Z \subset R^{d_Z}$, where $d_Z \leq d_Y$, using an encoder E_Y, and reconstructed with a decoder D_Y, such that $y \approx E_Y(z)$ when $z = D_Y(y)$, for all $z \in Z$.

Given a collection of inputs from X with corresponding profiles from Y, applying empirical PCA on these profiles yields the principal components (encodings) z and defines a decoder operator $D_{PCA}(z) = z\mathbf{V}^T$, where $\mathbf{V}$ is the eigenvector matrix calculated by the empirical PCA. In this framework, the encoder $\xi : X \to Z$ emerges, a transformation that compresses the input space X into the reduced PCA space Z, capturing the essential features of the available data. We approximate this encoding process ξ with a neural network ζ. The loss function $\mathcal{L}$ combines weighted root mean square error (WRMSE) and functional root mean square error (FRMSE): $\min_\zeta \mathcal{L} = w_s \underbrace{\left(\sum_{i=1}^{n}\sum_{j=1}^{d_z} v_j\left(\hat{z}_{ij} - z_{ij}\right)^2\right)}_{WRMSE} + \underbrace{\left(\frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{d_Y} w_p\left(\hat{Y}_{ij} - Y_{ij}\right)^2\right.}_{FRMSE}$

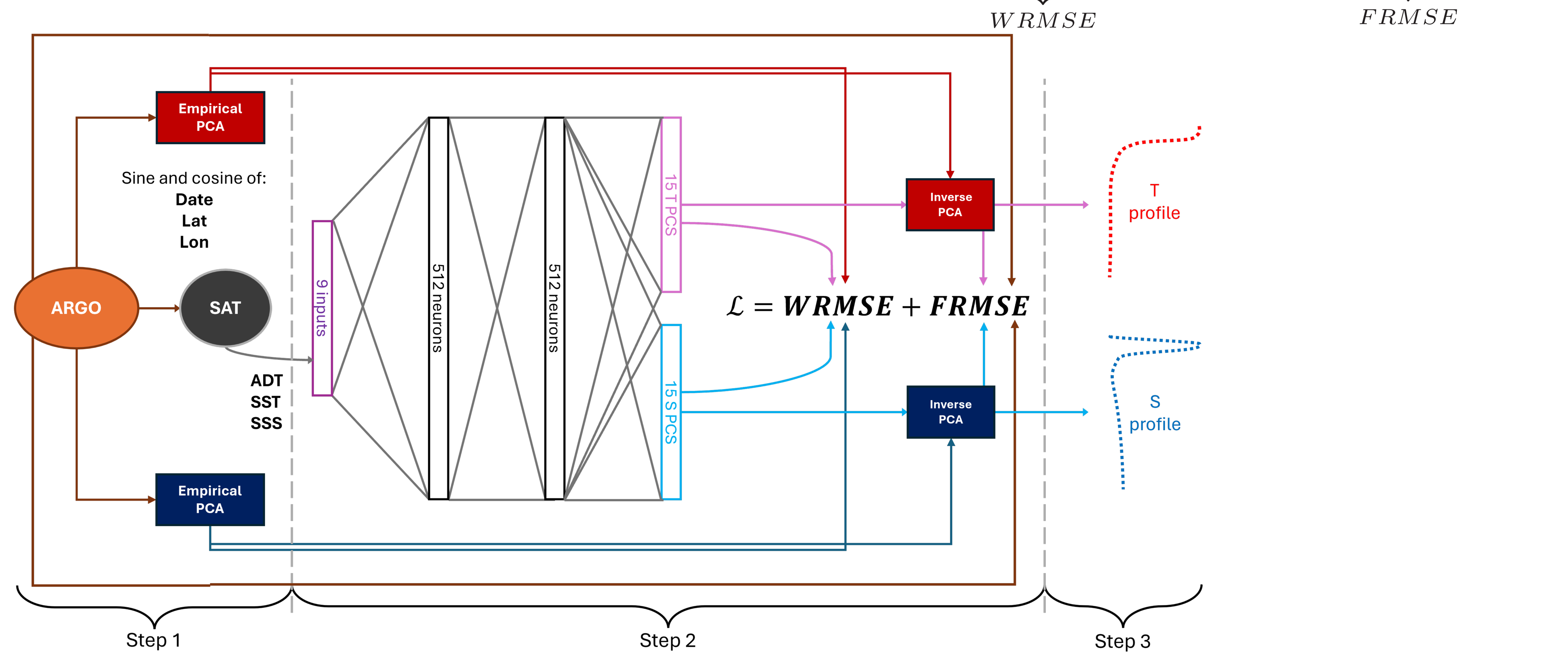

Figure 2: General diagram of our methodology. Step 1 computes the empirical PCA of the ARGO database. Step 2 trains a multilayer perceptron (MLP) from interpolated SST, SSH and SSS satellite observations, and harmonics of latitude, longitude and day of the year to predict the 15 Principal Component Scores (PCS) of T and S, which represent over 99% of the variance of the original data. Step 3 reconstruct the profiles via the inverse PCA operation. The MLP consists of 2 fully connected layers with 512 neurons, ReLU activation, and a 20% dropout rate. Inputs include interpolated SSH, SST, and SSS data, and the output approximates PCS for temperature and salinity profile reconstruction. Training uses 70% of the profiles, validation 15%, and testing the remaining 15%. The training process involves up to 8000 epochs, a batch size of 300, and early stopping based on validation loss improvement.

Results

We analyze the performance of NeSPReSO with respect to the 621 Argo profiles in our test set (not used in training), and compare its performance against GEM and ISOP methods. ISOP utilized profile-derived ADT and SST, unlike the other methods which use satellite data. This distinction favors ISOP in the upper ocean.

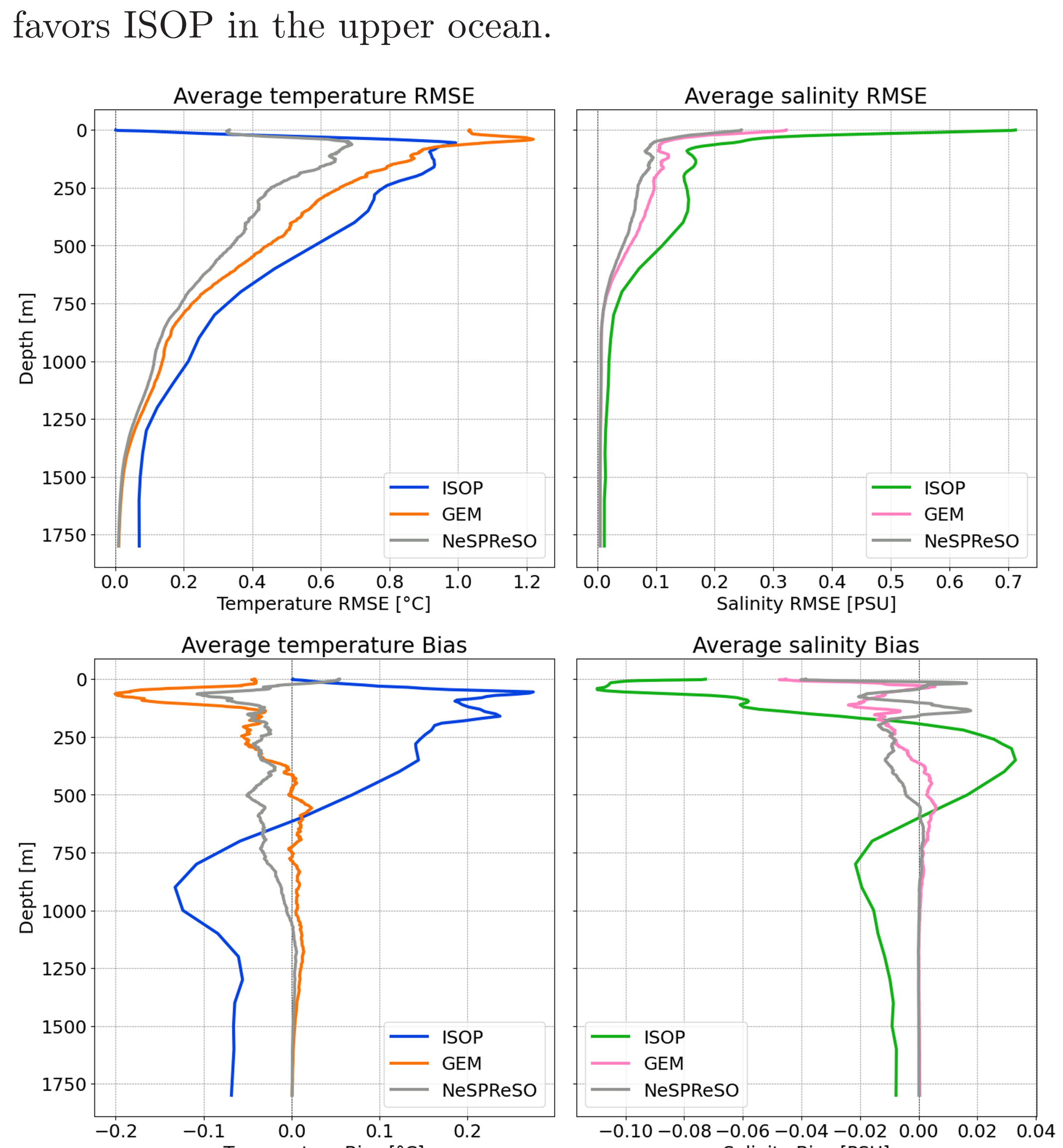

Figure 3: Average temperature and salinity RMSE and bias per depth. NeSPReSO outperforms GEM in temperature prediction across all depths and ISOP below 30 meters. While direct surface comparisons with ISOP are challenging due to its use of Argo SST, NeSPReSO provides more accurate temperature profiles, likely due to satellite SST usage. All methods show comparable temperature bias, indicating similar systematic errors. For salinity, NeSPReSO shows lower RMSE and bias across most depths, highlighting its superior accuracy in salinity prediction.

Crossing	Temperature RMSE	Temperature Bias	Temperature R^2	Salinity RMSE	Salinity Bias	Salinity R^2
Poseidon 1	0.586	0.031	0.996	0.118	-0.011	0.982
Poseidon 2	0.553	-0.207	0.998	0.111	-0.035	0.986
Campeche	0.524	0.079	0.996	0.069	0.017	0.992
Intense LCE	0.730	-0.133	0.996	0.105	-0.047	0.991

Table 1: RMSE, bias and R^2 between observations and synthetics across mesoscale eddy crossings. RMSE and bias values agree with the ARGO statistics for the same depth range, and R^2 is similar to the variance captured by the PCA.

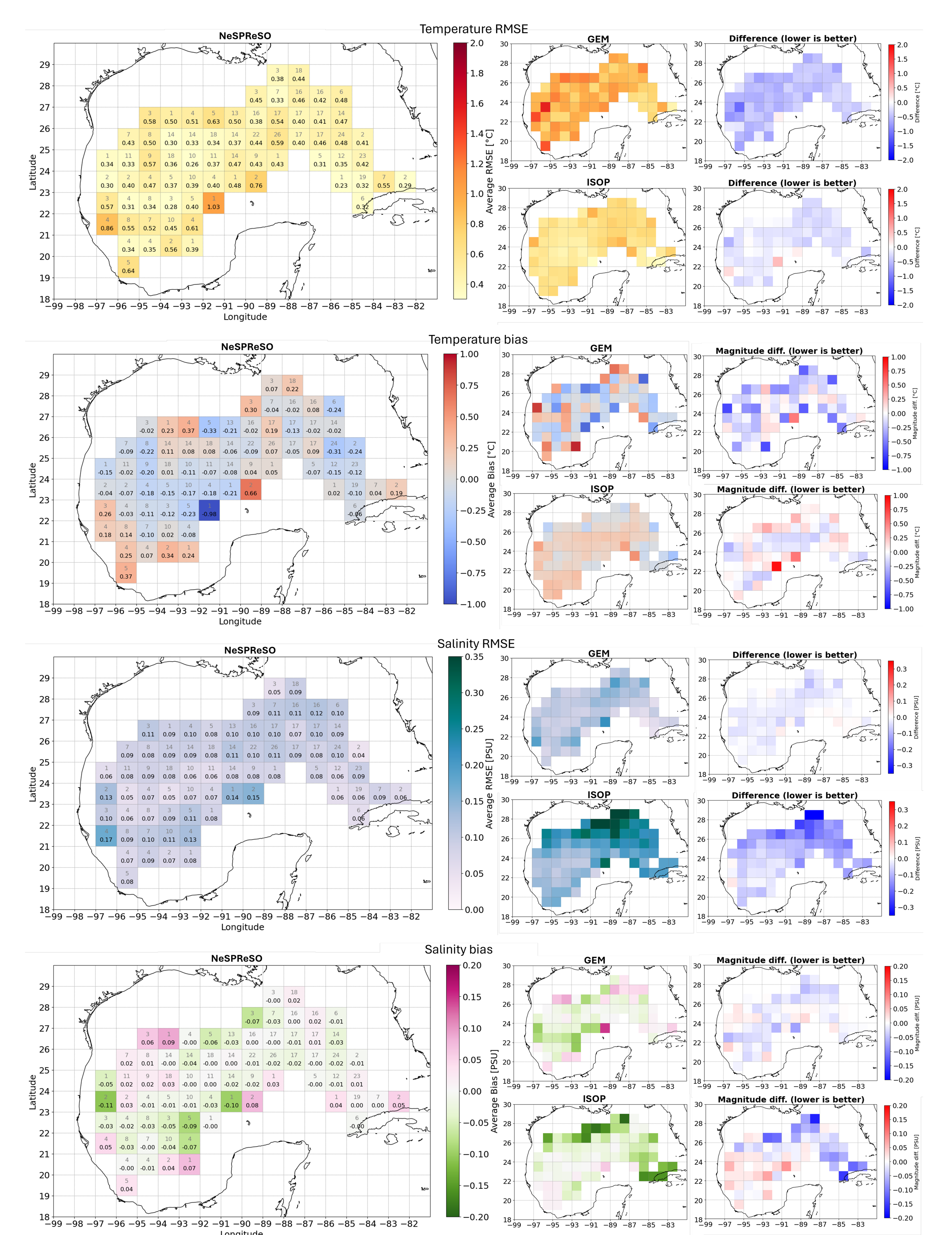

Figure 4: Spatial distribution of RMSE and bias for T and S, calculated using predictions at the same depths as ISOP for a fair comparison. NeSPReSO displays a lower overall RMSE for both T and S predictions for most regions across the GoM. NeSPReSO appears to have no predominant bias, and magnitudes comparable to the other methods or better.

Conclusion and future work

This work highlights ML's skill to synthesize temperature and salinity profiles from surface ocean data. Using PCA and NN, our model produces a better representation of the temperature and salinity profiles in the Gulf of Mexico compared to GEM and ISOP.

These results raises several questions that warrant further investigation. For instance, how will NeSPReSO perform in different oceanic regions with distinct hydrodynamic and thermohaline characteristics, and what adaptations might be required for different regional applications? Also, how can NeSPReSO be adapted and trained to effectively generate accurate temperature and salinity profiles in oceanic regions with depths shallower than the model's current maximum depth range? Future work will focus on addressing these questions, and improve further.