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COVER SHEET

An explainable machine learning prediction system for early-warning of heat stress on Florida's Coral Reef

Marybeth C. Arcodia[1], Richard Karp[2], Elizabeth A Barnes[1]

1 Department of Atmospheric Science, Colorado State University

2. Cooperative Institute of Marine and Atmospheric Science

University of Miami-Miami, Florida USA

Corresponding author: Marybeth Arcodia (marcodia@rams.colostate.edu)

Richard Karp (rkarp@earth.miami.edu)

Elizabeth A Barnes (eabarnes@colostate.edu)

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Key Points

- A data-driven, localized prediction system is developed for timing of moderate heat stress along Florida's Coral Reef
- The most important predictors across reef sites and prediction leads are identified using explainable AI
- Skillful prediction of heat stress onset up to six weeks in advance is achieved to provide valuable early warning for reef managers

Abstract

Coral reefs are facing increasing threats from rising ocean temperatures, necessitating timely and localized prediction tools to inform reef management and conservation. This study introduces a machine learning framework capable of forecasting the onset of moderate coral heat stress at site-specific resolution on Florida's Coral Reef. Leveraging the XGBoost algorithm, the data-driven prediction system forecasts whether heat stress will occur in a given season and, if so, the week in which moderate stress will begin. The prediction system achieves skillful forecasts up to six weeks in advance with a mean absolute error of approximately ±1 week. Two baselines are defined to compare performance– a multiple logistic regression model and a frequency-based model that predicts onset using the most common onset week, with the number of predicted onsets matched to the historical onset rate through random sampling. At the three reef sites analyzed, the machine learning model outperforms both baseline approaches in overall performance, including accuracy in predicting the timing of heat stress onset. Our approach uses the explainable AI technique, SHAP, to identify the most influential predictors across reef sites, lead times, and onset occurrence. Surface air temperature consistently ranked as a top predictor, while other key variables varied by location and lead time, underscoring the importance of localized analysis for drivers of heat stress onset. This framework provides an explainable tool for predictions on actionable timescales for anticipatory conservation with insight into stress onset at specific reefs, potentially allowing managers to develop reef-specific monitoring for emergency actions.

Plain Language Summary

Coral reefs are under growing threats from rising ocean temperatures, which can cause reef decline and widespread coral bleaching. This study developed a machine learning prediction tool that gives reef managers early warning about if and when moderate heat stress is likely to begin at specific reef sites along Florida's Coral Reef. The model is capable of forecasting the timing of heat stress up to six weeks in advance, with an average error of about one week—providing reef managers with valuable lead time to prepare. At the three reef sites analyzed, the machine learning prediction tool outperformed traditional methods, offering more accurate predictions of whether heat stress will occur and when it will start. By identifying which environmental factors are most important at each site through explainable AI, this tool offers insight for managers with information to focus monitoring and response efforts where and when they are needed most. These early warnings can be used to trigger emergency actions, such as increasing monitoring or deploying interventions, supporting more proactive and locally tailored reef conservation.

1. Introduction

Coral animals are the foundation of coral reefs, providing essential marine habitats, supporting approximately 25% of marine species (Fisher et al., 2015; Spalding et al., 2001). These reefs play a crucial role in protecting coastlines by reducing wave energy by up to 97% (Ferrario et al., 2014) and they contribute billions of dollars annually to the South Florida economy through ecosystem services such as fisheries, jobs, tourism, and flood mitigation (Brander et al., 2007; Johns et al., 2001; Storlazzi et al., 2019). However, corals are in decline due to various human-induced stressors, including overfishing and pollution (Jackson et al., 2014). While these stressors have caused initial declines, other factors such as ocean warming, coral diseases, and lack of recruitment have hampered natural recovery and led to declines of more than 80% of coral cover (Alvarez-Filip et al., 2022; Aronson & Precht, 2001; Cramer et al., 2020; Eddy et al., 2021; Gardner et al., 2003; Harper et al., 2023; Hughes, 1994; Williams et al., 2008).

Coral bleaching, associated with warm ocean temperatures, results in the expulsion of symbiotic algae that can supply more than 95% of a coral's energy needs, which can lead to reduced growth or reproductive capacity (Falkowski et al., 1984; Glynn, 1993). Although weakened, corals affected by bleaching may survive if temperatures decrease, but they are left vulnerable to future diseases and physiological impairment (Fisch et al., 2019; Miller et al., 2009; Neal et al., 2017). In the Florida Keys and wider Caribbean region, bleaching events are becoming more frequent and severe (Manzello, 2015; van Hooidonk et al., 2016), which has led to 22 Caribbean corals listed as threatened under the Endangered Species Act (NOAA Fisheries, 2022). To combat coral decline, coral restoration has emerged as a strategy to conserve key reef-building species throughout the Caribbean (Boström-Einarsson et al., 2020; Lirman & Schopmeyer, 2016; Young et al., 2012). Heat-related stress on corals was exacerbated during the 2023 South Florida marine heatwave, which caused the most severe heat stress on record in the Florida Keys (Neely et al., 2024; Williams et al., 2024), and impacted key coral species used in restoration. In response, restoration practitioners quickly mobilized to conserve these species and genetic material by providing emergency measures such as shading and relocation to land-based facilities. These actions demonstrate that emergency action plans can be implemented in real-time to minimize the impact on corals during extreme marine heat waves. Therefore, predictive tools for heat stressors can guide proactive coral reef conservation and management.

Currently, the National Oceanic and Atmospheric Administration Coral Reef Watch (NOAA CRW) monitors threats to global coral reef environments, providing alerts and outlooks to reef managers via a publicly available website (https://coralreefwatch.noaa.gov/; Liu et al., 2014). In particular, CRW produces bleaching alerts at various levels based on the daily sea surface temperature forecasts from the dynamical forecast model, NCEP CFSv2 (Saha et al., 2014). CRW constructs multiple ensemble members from the CFSv2 forecasts to produce weekly probabilistic outlooks for the likelihood of coral heat stress up to four months in advance (Liu et al., 2018). They issue regional warnings and alerts based on accumulated heat stress in an area at both the 90% and 60% level for 5 heat stress alert levels. Heat stress is measured primarily through the metric “degree heating weeks” (DHWs), quantified as the accumulated heat stress in an area over the past 12 weeks. When DHWs reach 4^{o}C-weeks, the corals are exposed to moderate heat stress and significant coral bleaching is likely. This moderate heat stress threshold does not necessarily equate to coral bleaching or coral death, but is a critical threshold for monitoring risk as higher DHWs often signify reef-wide bleaching and high mortality (Hughes et al., 2018).

Although the CRW forecasts provide a valuable outlook for the global coral community, the bleaching alerts and outlooks are based solely on the CFSv2 dynamical forecasts of sea surface temperature. CRW notes that the accuracy of the CFSv2-based prediction system varies by region, performing best in areas influenced by large-scale climate patterns like the El Niño Southern Oscillation ENSO in the tropical Pacific Ocean (Saha et al., 2014), while remaining limited by model physics, initialization uncertainty, and the inherent unpredictability of the climate system (Liu et al. 2017). Machine learning methods have emerged as a useful tool for overcoming limitations of purely dynamical prediction systems, particularly for localized sea surface temperature forecasting on short-range timescales (Bonaglia et al., 2025; Cohen et al., 2019; Ibebuchi & Obarein, 2025). More specifically, machine learning has been used for early warning prediction of bleaching events with promising skill over conventional prediction schemes, such as in Taiwan (Lin et al., 2023) and the Coral Triangle (Eshwar et al., 2024; Novi & Bracco, 2022). However, a localized machine learning approach has not been applied specifically for early warning forecasting of bleaching-related heat stress in Florida's Coral Reef.

Here, we train a machine learning model to predict both *if* and *when* three Florida Keys coral reef sites will experience an onset of moderate heat stress (≥4.0 DHW) each summer at lead times from 0-6 weeks. Using a combination of both site-specific and large-scale environmental predictors, the data-driven prediction system produces skilfull localized forecasts of stress events. Further, we incorporate explainable AI methods to reveal the most important predictors at each site for each prediction. The explainability features of the model allow us to move beyond the so-called "black box" notion of the machine learning prediction model to gain insight and build trust in the predictive capabilities of the data-driven approach. The model developed in this study is capable of making skillful predictions of coral-related heat stress on actionable timescales to aid in conservation efforts along Florida's Coral Reef.

2. Data and Methods

2.1 Data

Weekly data from 1985-2024 are taken from the NOAA Coral Reef Watch website (https://coralreefwatch.noaa.gov/) at 5km resolution centered on three coral reefs along Florida's Coral Reef: Sand Key (24.46° N, 81.88° W), Sombrero Reef (24.63° N, 81.11° W), and Molasses Reef (25.02° N, 80.38° W) (Figure 1a). Data from each site include the weekly-mean HotSpot value, the Degree Heating Week (DHW), and the mean sea surface temperature (SST) anomaly. The HotSpot and DHW are terms used by NOAA Coral Reef Watch (Skirving et al. 2020) to assess localized heat stress. The HotSpot is a measure of the occurrence and magnitude of the instantaneous heat stress that causes coral bleaching, measured by the number of SST degrees above the monthly mean maximum. The DHW is a measure of how much heat stress has accumulated in an area over the past 12 weeks. It ranges from 0-20 ^{o}C-weeks where 1 DHW is equal to 1 week in which the SST exceeded 1^{o}C over the maximum monthly mean SST in that grid cell with 20 ^{o}C-weeks resulting in near complete mortality. NOAA Coral Reef Watch deems a DHW of 4^{o}C-weeks as moderate heat stress that indicates a risk of coral bleaching. Onset of moderate heat stress in this study is thus defined as the week in which the DHW will reach a value of greater than or equal to 4^{o}C-weeks. A timeseries of DHW at Sombrero Reef is shown in Figure 1b and a histogram of the frequency of the week in which onset of moderate heat stress occurred in Figure 1c.

We aim to predict the number of weeks until the onset of moderate (or higher) heat stress, defined when the DHW is greater than or equal to a value of 4.0. Predictors include both site-specific inputs as well as regional and global climate variables (Fig. S1). The site-specific predictors include the DHW, HotSpot, and SST anomaly values at the time of prediction, and the DHW lagged by 1 week and the DHW lagged by 2 weeks to include the temporal evolution of stress onset. These data are taken from the NOAA Coral Reef Watch Single Pixel Stations at a 5km resolution (Skirving et al., 2020).

The regional and global predictors include surface air temperature, downward solar radiation flux, low-level zonal wind, Loop Current Index, the ENSO ONI Index, and the week of year at the prediction initialization. The surface air temperature and downward solar radiation flux (1000mb) and low-level zonal wind (925mb) are taken from the NCEP-DOE Reanalysis 2 (Kanamitsu et al., 2002) as daily data and averaged to weekly data at the grid cell closest to the reef sites (25N; 280E). The Loop Current Index is calculated using NOAA OI SST V2 High Resolution dataset (Huang et al., 2021; 0.25 degree grid) as the area-averaged (21N-28N; 270-281E) weekly SST anomalies. The ENSO Index is computed using the NOAA ERSST V5 (Huang et al., 2017) for the 3-month running mean of ERSST.v5 SST anomalies in the Niño 3.4 region (e.g. ONI Index) and linearly interpolated to weekly values. The predictors selected include those that have been previously demonstrated to influence sea surface temperatures and potential coral heat stress in the Florida Keys (Barnes et al., 2015; Kourafalou et al., 2018; Lachs et al., 2021; Skirving et al., 2017; Spillman et al., 2011). Additional local and global predictors were explored but were not found to notably improve skill through feature selection ranking; a list of additional variables tested can be found in Table S2.

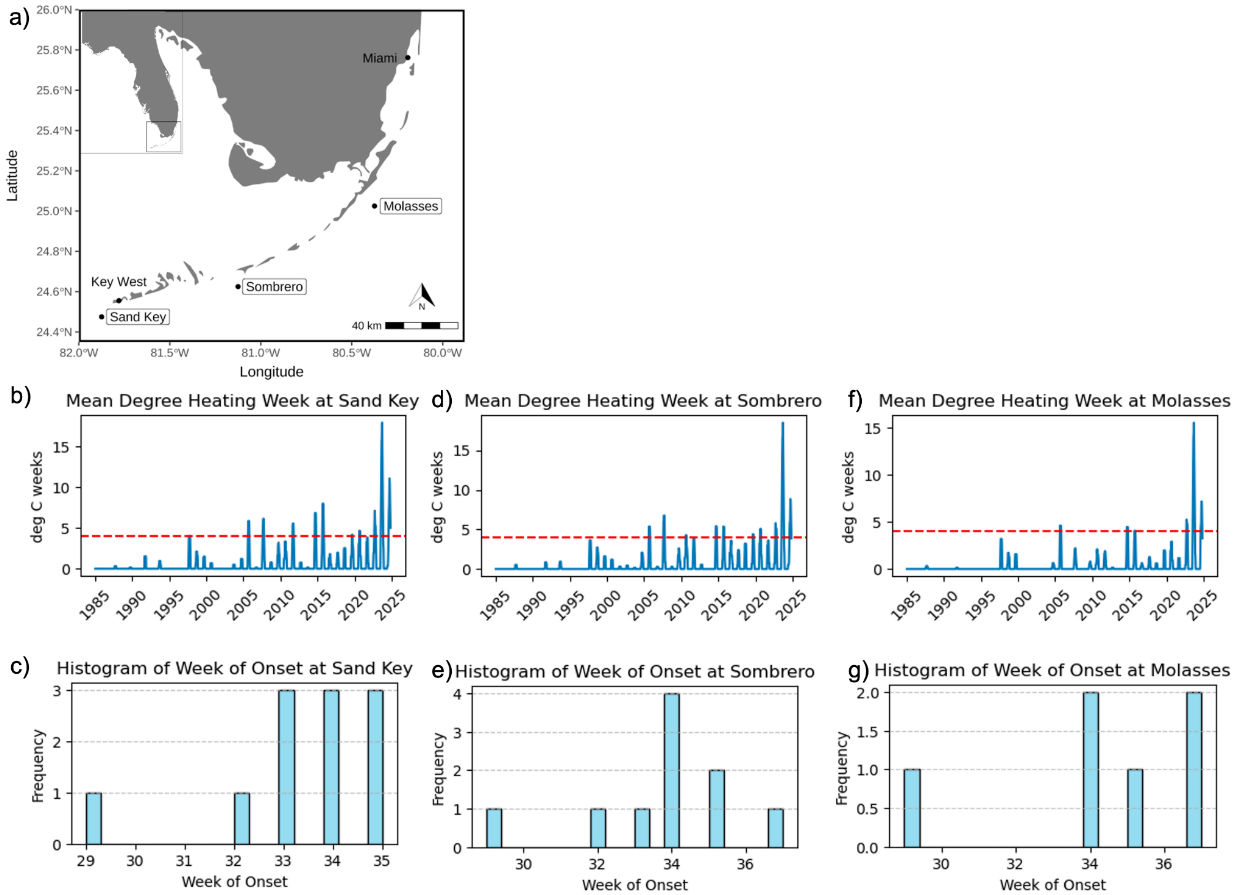

Figure 1. a) Inset map of the Florida Peninsula for the three reef site locations on Florida's Coral Reef: Sand Key, Sombrero Reef, and Molasses Reef. b,d,f) The mean degree heating week (DHW) in ^{O}C-weeks from 1985-2024 for each reef. The red dashed line at y=4 indicates moderate stress. c,e,g) Histogram showing the frequency of the onset week-of-year for moderate stress.

2.2 Machine Learning Model

The goal of this study is to predict if and when onset of moderate heat stress will occur at each reef site (e.g. number of weeks until DHW≥4^{o}C-weeks). The machine learning model used is the XGBoost Random Forest Classifier (Chen & Guestrin, 2016). XGBoost (Extreme Gradient Boosting) is an efficient and powerful gradient boosting algorithm that builds ensembles of decision trees sequentially to incrementally improve predictions, demonstrating success for climate forecasting from timescales of days to months (Bhoopathi et al., 2024; Deng et al., 2025; Qian et al., 2020). The parallel processing and tree-pruning qualities of XGBoost allow it to learn complex and nonlinear relationships in data, while also allowing for understanding of the model's predictions through explainability techniques. A schematic of the machine learning setup, including the predictors and predictands, is shown in Figure S1.

Only weeks 21–40 of each year are used for prediction, as these are historically the warmest months when heat stress occurs (Figure 1c,e,g). Given the predictors for each week (Section 2.1), the model classifies the prediction into one of seven categories: the integers ranging from 6 to 0 weeks until onset (with 0 indicating onset has occurred) or no-onset. After onset has occurred, the model is trained to predict the 0 weeks until onset class until the end of the season. The model can continue to update its prediction each week, even if it had previously predicted no-onset for that season.

Onsets of moderate heat stress only occurred 11 summers at Sand Key, 10 summers at Sombrero Reef, and 6 summers at Molasses Reef in the full 40-year dataset (Figure 1). Due to anthropogenic climate change and rising sea surface temperatures, onsets have occurred more frequently at each reef site in the most recent decade (Burns et al., 2024). Thus, the data is imbalanced and skewed towards no-onset prediction, and the imbalance is not evenly split amongst the temporally correlated time series data. To combat this, we use a cross validation approach in which training and testing data is split into 5-folds. The test data is split into 8-year sequential chunks with the remaining data used for training (Table S1). Furthermore, we implement a custom weighted loss function such that no-onset predictions are weighted as 0.02 with all onset predictions weighted at 1.0. The model is optimized by minimizing the negative multinomial log-likelihood loss function. The softmax activation function is applied to convert the outputs (logits) to probability estimates, such that the class with the highest probability is selected as the prediction. The other hyperparameters were selected through an iterative hyperparameter sweep to find the combination of parameters across the training data for all 5 training folds that resulted in the highest F1 score for each reef site (information about scores in Section 2.3). A table of the hyperparameters used and the results from the sweep are found in Table S3 and Fig. S2.

2.3 Skill Assessment

Skill metrics were used to evaluate model performance comprehensively for both years in which onset did and did not occur (Figure 2). We use standard classification metrics to evaluate the model's ability to predict stress occurrence and onset timing. We assign a correct positive (hit) as a correctly forecasted onset and a correct negative as a correctly forecasted no-onset. These metrics are similar to those from a contingency table with labels of onset and no-onset, as used in similar analyses to classify bleaching predictions (DeCarlo, 2020; van Hooidonk & Huber, 2009). A tolerance of ±1 weeks is used in skill assessment (e.g. if onset was predicted in 3 weeks, but the true timing was 4 weeks, this is counted as correct), as the relative timing still allows conservationists to make adequate preparations for onset of heat stress while accounting for uncertainties in the predictions.

We summarize six skill metrics:

- *Onset accuracy*: number of correct predictions for an onset week within ±1 week of true onset divided by the total number of valid onset week predictions; also called the *recall*
- *No-onset accuracy:* number of correct predictions for no-onset divided by the total number of valid no-onset week predictions
- *False alarm*: the number of predictions for which the model predicted an onset, but no onset occurred, divided by the total number of valid no-onset week predictions
- *Missed onset:* number of predictions for which onset occurred, but the model predicted it either sooner or later than it did occur by more than the tolerance of 1 week divided by the total number of valid onset week predictions
- *Precision:* the number of correct onset predictions divided by the total number of correct onsets plus false alarms.
- *F1 score:* the overall metric for model performance – the harmonic mean of the precision and recall scores, taking into account performance for predicting both the if and when of stress onset; computed as

$$2 * \frac{precision * recall}{precision + recall} \tag{1}$$

An F1 score of 1 indicates perfect predictions (exactly correct), while 0 indicates no skill. A metrics table is included in Table S4 for each reef site with the numerics for computing the scores. All metrics are computed on the test data corresponding to each training fold and the final reported value is the average over all test data folds. We note that all predictions made for weeks after an onset occurred in a season are excluded from the skill computations to avoid artificially inflating skill scores.

To further evaluate the prediction skill specifically for those years in which heat stress occurred, the mean absolute error is computed for each onset prediction class (i.e. 0-6 weeks until onset; see Figure 3). The mean absolute error is computed as the absolute value of the difference between the predicted number of weeks until onset and the true number of weeks until onset.

2.4 Baselines

The performance of the XGBoosted Model is compared to two baselines as reference points for evaluation of model skill: 1) a frequency model and 2) a multiple logistic regression (linear) model. We train separate models (XGBoost, multiple linear regression, and frequency) for each of the three reef sites to tailor the model architecture to localized predictions. The frequency model baseline is constructed by first analyzing the full 40-year dataset to identify the week in which onset most frequently occurred (Fig. 1c,e,g). Next, we calculate the total number of seasons in which onset occurred, regardless of the specific week. The model randomly selects that number of seasons and assigns the most frequent onset week to each, while the remaining seasons have all no-onset predictions. For example, at Sombrero Key, week 34 was the most frequent week for moderate stress onset out of the 10 seasons that stress occurred out of the full 40-season dataset (see Fig. 1c). The frequency model thus predicts week 34 for stress onset for 10 randomly selected seasons, with the predictions for the remaining seasons classified as no-onset. For reef sites in which multiple weeks tied for the most frequent onset week, the earlier onset week is chosen.

The frequency model provides a meaningful benchmark because it reflects the underlying tendency of the system without incorporating any dynamic or environmental predictors. By reproducing the historical onset rate and timing using only the frequency distribution, it allows us to assess whether more complex models provide skill beyond what can be achieved by simply relying on historical patterns. Further, the frequency model could be considered a simple, but conservative baseline as it includes knowledge of the full-time series, while the XGBoost and logistic model withhold some training data for testing of the model performance.

A multiple logistic regression is also compared to the XGBoost model performance. This linear model uses the same inputs and custom weighting as the XGBoost model, and the data is split using the same cross-validation folds. Our use of a linear model baseline allows us to assess how much predictive skill can be achieved by assuming linear relationships between predictors and onset timing. Improvements in performance by the XGBoost model can thus be attributed to the XGBoost's ability to capture nonlinear interactions and complex feature combinations that a linear model cannot represent.

A direct skill comparison with the Coral Reef Watch Outlook is not possible at the individual reef scale, as the CFSv2 SST forecast provides only broad seasonal maps of root mean square error and correlation, without assessing its ability to predict the timing of heat stress onset. Because no existing operational product evaluates onset timing skill at the site level for the Florida Keys, we establish our own baselines to meaningfully assess model performance in a localized context.

3. Results

3.1 Model Performance

We assess the skill of the three models (XGBoost, linear, and frequency) in predicting if and when moderate or higher heat stress will occur at Sand Key, Sombrero Reef, and Molasses Reef. Skill is assessed for every week that a prediction is made, e.g. 20 weeks per season for the full 40-year dataset. We exclude weeks following onset from skill metric calculations, as predictions during this period would be artificially inflated—onset (0 weeks) is directly defined by the DHW input feature, offering no real predictive skill. Including these weeks would also be of limited value to managers, who require advance warning of heat stress, not confirmation after it has occurred.

At all three reef sites, the XGBoost model outperforms both baseline models as reflected by the higher F1 scores in Fig. 2a (see Table S4 for additional metrics for precision and recall). We use the F1 score for evaluation of overall performance since the F1 score strikes a balance between precision and recall. It accounts for both how often the model predictions of onset were actually correct (precision) and how many actual onsets the model managed to accurately predict (recall). At Sand Key, the F1 score is 0.56, while the F1 score for the linear and frequency models are 0.19 and 0.35, respectively. Furthermore, given the tolerance of ±1 week, the onset accuracy is approximately 70% at Sand Key and Molasses Reef, and jumps to over 80% at Sombrero Reef. The accuracy for no-onset predictions is over 80% at all three reef sites for the XGBoost model. The XGBoost model has the lowest missed onset rate of the three reef sites compared to the baseline models and a lower false alarm rate, except at Molasses Reef.

The higher performance of the machine learning model compared to the logistic regression model suggests that the system exhibits nonlinear relationships, which the machine learning model is better able to capture. Further, the linear model generally performs better than the frequency model, likely due to its incorporation of local and global predictors beyond only the historical onset timing.

We additionally evaluate skill for a tolerance of ±0 weeks, meaning prediction for exact timing of onset (Fig. S3, Table S5). As expected, the skill drops across all metrics for all three models at all reef sites. However, the XGBoost model is skilfull and consistently outperforms the two baselines.

Figure 2. Prediction performance for all predictions for the XGBoosted Random Forest model (XGB; pink), the Logistic Regression model (linear; gray) and the Frequency model (frequency; green) for the three reef sites for 1-week tolerance. The bar plots show the F1 score (a), onset accuracy (b), no onset accuracy (c), false alarm rate (d) and missed onset rate (e).

We also assess the mean absolute error for the predicted weeks until onset for those years in which moderate heat stress occurred. The XGBoost and linear model have comparable mean absolute error of approximately 1 week out to 6 weeks until onset (Fig. 3), revealing skillful predictions on actionable timescales in which necessary preparation measures and resource allocation can take place.

The frequency model underperforms at most leads compared to the XGBoost and linear model. Decreases in error at longer lead times for the frequency model are largely due to fewer predictions in those categories. In contrast, shorter lead times (e.g., 0–2 weeks) allow for a wider range of possible predictions, increasing potential error. This linear increase in skill with time behavior is a structural artifact of the frequency model and is not observed in the other two models.

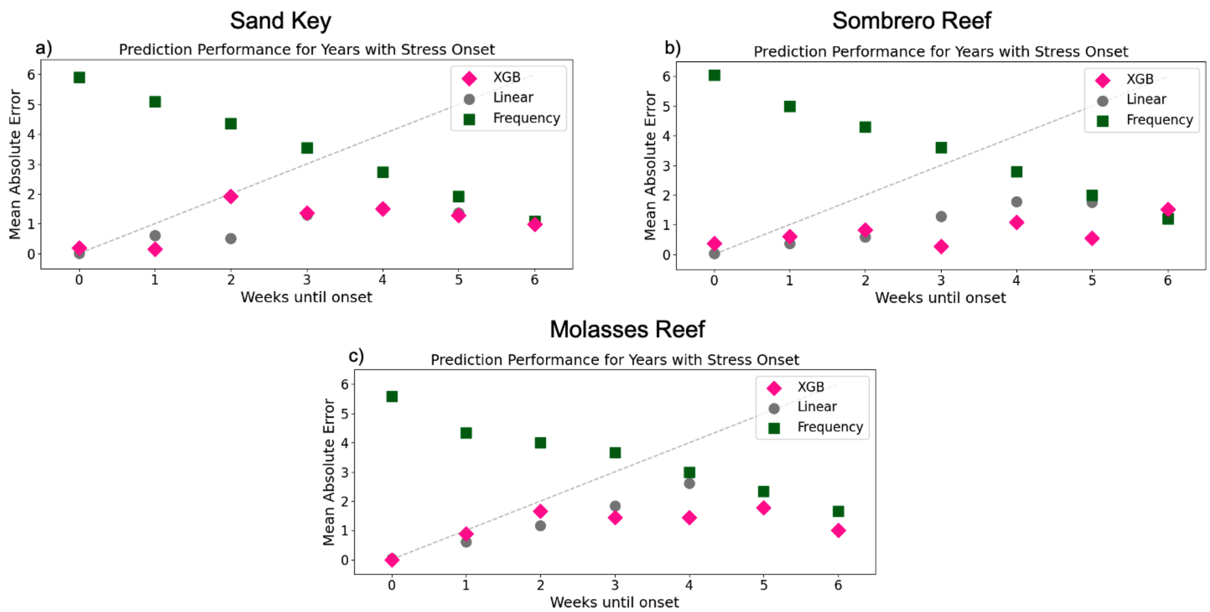

Figure 3. Prediction performance only for years with stress onset for a) Sand Key, b) Sombrero Reef, and c) Molasses Reef. Mean absolute error of the prediction week is plotted as a function of the true weeks until stress onset, with the gray dashed line representing a 1:1 line, for the XGBoosted Model (XGB; pink diamonds), the logistic regression model (linear; gray dots) and the frequency model (frequency; green squares).

3.2 Explainable AI

After evaluating the model performance and concluding that the XGBoost model performs sufficiently well for predicting both if and when moderate heat stress will occur, we seek to explore the models' decision making processes. We utilize explainable AI to provide transparency into how the XGBoost models incorporate the input features into the predictions, which provides insight to build trust and confidence in the model output (McGovern et al., 2019). Here, we use the explainable AI technique of SHAP, or SHapley Additive exPlanations– a game theory-based method that quantifies the contribution of each feature to a model's prediction (Shapley, 1953). SHAP values allow us to interpret how individual input features drive predictions by assigning each feature a positive or negative impact on the output. Computing and interpreting SHAP values enables us to gauge the trustworthiness of the model and validate our machine learning model (Deng et al., 2025; Kiefer et al., 2023; Leinonen et al., 2023; Lundberg & Lee, 2017). Further, SHAP provides global and local interpretability to understand both overall feature importance and specific predictions.

SHAP values for Sand Key Reef are shown in Fig. 4. SHAP values are computed individually for each prediction class and averaged across all folds. The base value shown for each class is the average model output (logit) for that class across the training data before seeing any input features. These base values serve as class-specific reference points, such that the more positive the value, the more likely the class is to be chosen and vice versa. The SHAP values explain how each feature shifts the model's output from its base value toward the final prediction for that class. Simply put, the SHAP values then can be interpreted as increasing or decreasing the probability of a particular class being predicted.

Moreover, input features are ranked in order of importance from top to bottom for each class. The ranking of important input features varies from the no-onset to onset predictions and based on the number of weeks predicted until onset. The HotSpot and DHW values rank as consistently important predictors, particularly for less weeks until onset, which is expected given the HotSpot and DHW value are both derived from the grid-cell SSTs which define the moderate heat stress level. The SHAP values also reveal that higher DHWs and higher air temperatures (purple dots) increase the likelihood of the 1-4 weeks until onset predictions (Fig. 4b-e). The model's use of these input variables align with our physical understanding in that higher DHW values and warmer air temperatures indicate higher likelihood of imminent stress onset, allowing us to build trust in our machine learning models. For the 5-6 weeks until onset classes (Fig. 4f-g), the air temperature ranks lower in importance with less of an overall influence on the ultimate prediction. The week of the year emerges as the most important predictor for 4-6 weeks until onset. The earlier in the season (i.e. lower value for the week of year), the more likely the model is to predict 4-6 weeks until onset, suggesting the model has learned that onset is more likely later in the season (as seen in Fig. 1c).

For predictions of no-onset (Fig. 4h), the DHW value and the surface air temperature rank as the most important predictors. We find that lower DHW values and colder air temperatures increase the probability of no-onset prediction. Further, the model ranks two regional/global predictors, the Loop Current Index and ENSO Index, as the next most important input features. Lower values of the Loop Current Index (i.e. cooler SST anomalies in the Loop

Current region) increase the probability of a no-onset prediction and vice versa. Lower values of the ENSO Index (indicative of La Niña conditions, or cooler SST anomalies in the tropical Pacific) increase the probability of no-onset, while higher values of the ENSO Index (indicative El Niño conditions, or warmer SST anomalies in the tropical Pacific) decrease the probability of a no-onset prediction. We find that both local and large-scale input features provide predictive information for the probability of onset occurrence in a season.

While the ENSO Index ranks as a highly important feature for the no-onset prediction class, it falls in the bottom half of important features for the 0-6 weeks until onset classes. We hypothesize this is due to the seasonal variability of ENSO's global impacts, such that ENSO plays a significant role in whether or not onset will occur in a season, but is less of a factor for the timing of heat stress onset at a weekly timescale. For the prediction class of 0 weeks until onset (Fig. 4a), the DHW values including the lagged DHW rank as the most important, while the other features have much less importance. Since the value of the DHW determines the onset, these feature rankings are expected and further strengthen our trust in the model.

We next assess the SHAP values at Sombrero and Molasses Reef (Figs. S4-S5) and find some similarities in the ranking of features as found in Sand Key. For example, the DHW and air temperature are found to be the most important predictors for the no-onset class (Figs. S4h-S5h). The Loop Current Index and ENSO Index rank highly for Molasses Reef, similar to Sand Key, but fall lower in importance at Sombrero Reef. The HotSpot, DHW, and air temperature values are important predictors for the 1-4 weeks until onset classes (with the exception of 2 weeks until onset for Sombrero Reef; Fig. S4c). The DHW and the lagged DHW values remain as the top predictors for the 0 weeks until onset class in both locations.

However, there are some key differences in the predictors that vary by class for the three reef sites. The downward solar radiation flux ranks as a more important predictor across the 1-6 weeks until onset classes at both Sombrero and Molasses Reef than at Sand Key. At Molasses Reef, the SST anomaly is a more highly ranked predictor than the other locations. Warmer SST anomalies increase the likelihood of onset prediction for sooner onset (<4 weeks until onset), while warmer SST anomalies decrease the likelihood for later onset (5-6 weeks until onset). The discrepancies in ranking of important features across reef sites highlights the need for localized predictions with both site-specific and regional/global predictors as each reef is impacted by different environmental factors on different timescales.

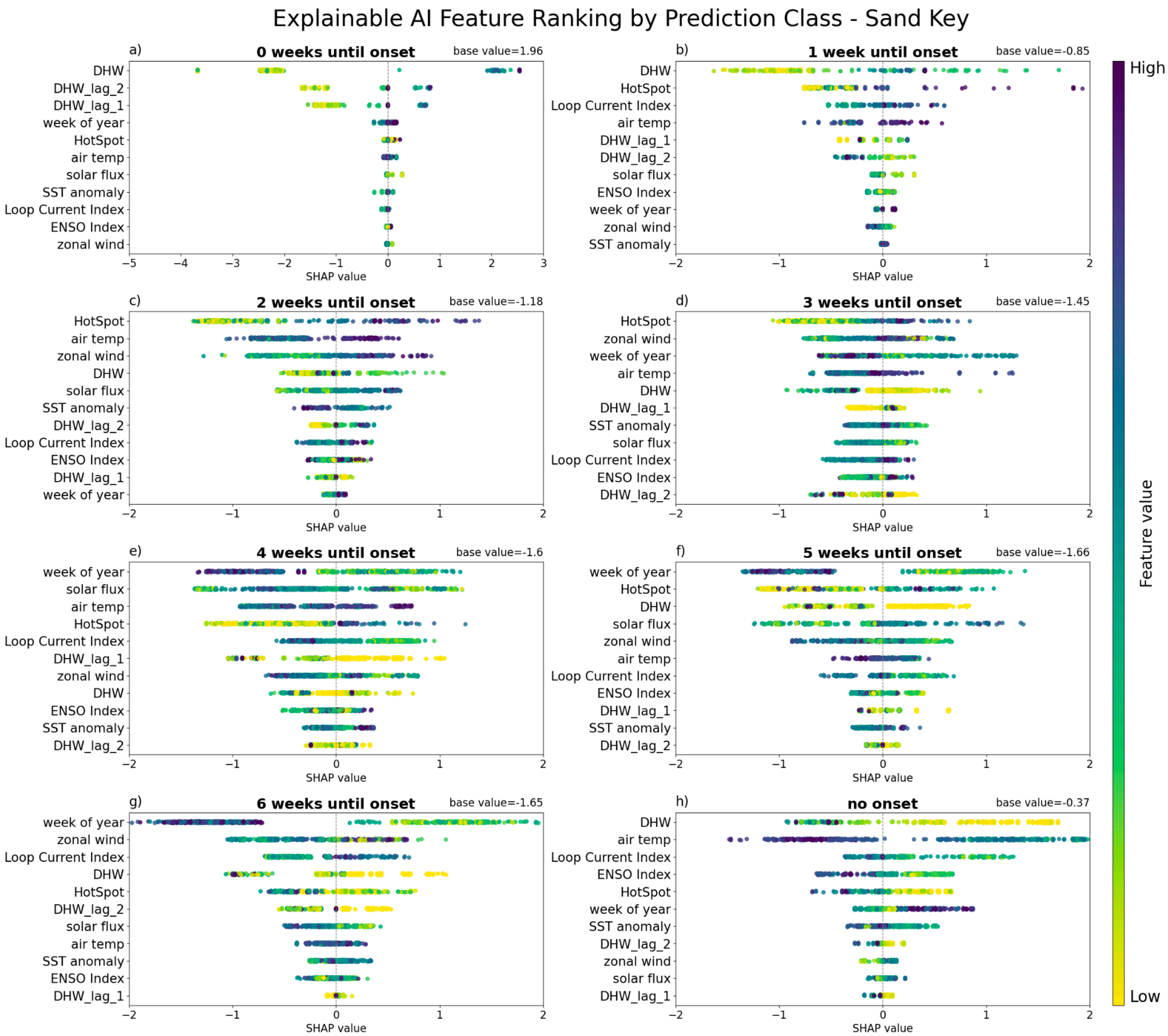

Figure 4. Shapley additive values for test years from all folds using k-fold cross validation (1985-2024) for Sand Key for each prediction class (a-h). The top predictor ranks as most important to the prediction and the bottom predictor is the least important. Purple values indicate higher magnitude of the variable and yellow colors indicate lower magnitude values. Dots with positive SHAP values indicate the predictor increased the probability of that class being predicted, while negative SHAP values indicate the predictor decreased the probability of that class being predicted. The base value, or expected value, for each class is the average model output for that class across all training data.

4. Conclusions and Discussion

This study presents a machine learning, site-specific prediction system capable of forecasting the timing of moderate coral heat stress events on Florida's Coral Reef. The framework determines whether or not heat stress is expected to occur in a given season, and if so, predicts its onset timing. At the three reef sites analyzed– Sand Key, Sombrero Reef, and Molasses Reef– the machine learning XGBoost model outperformed both baseline approaches (a multiple logistic regression model and a historical frequency prediction model). The XGBoost model achieved overall higher skill for both onset and no-onset accuracy, with lower rates of false alarms and missed onsets across the reef sites. Moreover, the XGBoost model achieved skillful predictions up to six weeks in advance, with a mean absolute error of approximately ±1 week for onset timing. Importantly, these predictions are made on operationally relevant timescales, offering a valuable tool for anticipatory coral reef conservation and management.

A key aspect of our machine learning framework lies in our use of the explainable AI technique, SHAP values, to identify the most influential predictors of heat stress onset at each site. By making model decision-making transparent and interpretable, explainable AI techniques like SHAP foster trust among scientists and conservation managers—shifting away from the traditional view of machine learning as a "black box" (McGovern et al., 2022). Notably, surface air temperature and SST-derived quantities (DHW and HotSpot) emerged as critical predictor variables across sites, underscoring the need to collaborate with conservation managers to ensure these parameters are captured by site-specific monitoring systems. However, other principal influential factors differed by reef site. For instance, the Loop Current and ENSO indices ranked as more important predictors at Sand Key and Molasses Reef than Sombrero Reef. Thus, the effects of large-scale climate patterns may be masked or enhanced by more local conditions at certain reef sites, highlighting the need for localized heat stress prediction.

At present, we consider the purely data-driven models developed in this study to be complementary to, rather than replacements for, existing operational systems such as NOAA Coral Reef Watch's probabilistic bleaching outlooks, particularly for advancing understanding of site-specific predictability. Indeed, some of our inputs are from NOAA Coral Reef Watch-derived data, and therefore highlight the necessity of this tool for evaluating regional temperature threats. This work provides a complementary and localized system, showcasing the potential of advanced data-driven tools to strengthen and diversify predictive capabilities beyond established products to better understand what is happening at high value reefs. Sombrero Reef, for example, is part of the NOAA Mission Iconic Reef project (https://missioniconicreefs.org/), which seeks to restore 25% coral cover at this site. Therefore, enhanced development of reef-specific models to predict bleaching stress throughout a season can allow managers and practitioners to prioritize response actions based on potential heat stress risk.

We also note here that while 4°C-week heat stress accumulation (DHW=4.0) is a strong predictor of coral bleaching, it does not guarantee that bleaching will occur at that reef location. Nevertheless, these tools can help managers prioritize and implement actions—such as interventions or increased monitoring—by establishing trigger points in emergency plans on a reef-by-reef basis. Transparent communication of prediction uncertainties and model limitations is necessary to better support decision-making under uncertainty in coral reef conservation.

Future work motivated from this study includes further enhancements of the data-driven prediction system and exploration of additional predictors. For example, sea surface height could be used to better capture the Loop Current evolution and advection of sea surface and subsurface temperature anomalies (e.g. Hiron et al., 2020). Applying this framework to additional reef sites would help expand the usability of the forecasts for conservationists monitoring many reef sites. Hybrid dynamical-machine learning approaches should be explored as a way to build upon current operational outlook systems like NOAA Coral Reef Watch. This study's development of site-specific predictions for both the occurrence and timing of moderate heat stress events, extending out to six-week lead times, demonstrates the potential of machine learning to support proactive reef management and lays the groundwork for more anticipatory, impact-driven conservation strategies.

Data Availability Statement

NOAA Coral Reef Watch 5km products can be accessed at https://coralreefwatch.noaa.gov/product/vs/data.php. NOAA OI SST V2 High Resolution Dataset data provided by the NOAA PSL, Boulder, Colorado, USA, from their website at https://psl.noaa.gov. NCEP/DOE Reanalysis II data provided by the NOAA PSL, Boulder, Colorado, USA, from their website at https://psl.noaa.gov. ONI data provided by NOAA Climate Prediction Center accessed at https://www.cpc.ncep.noaa.gov/data/indices/oni.ascii.txt.
The NOAA Mission Iconic Reef project can be accessed at https://missioniconicreefs.org/. All software and code will be made available via a public Zenodo repository.

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Supporting Information for

An explainable machine learning prediction system for early-warning of heat stress on Florida's Coral Reef

Marybeth C. Arcodia[1], Richard Karp[2], Elizabeth A Barnes[1]

1 Department of Atmospheric Science, Colorado State University

2. Cooperative Institute of Marine and Atmospheric Science

University of Miami-Miami, Florida USA

Corresponding author: Marybeth Arcodia (marcodia@rams.colostate.edu)

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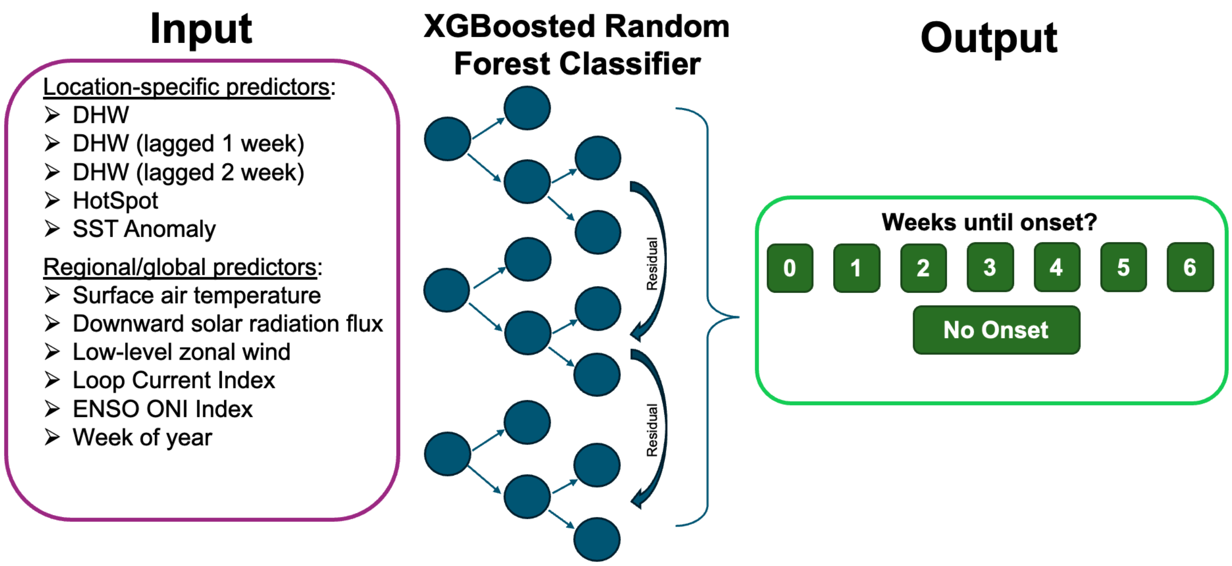

Figure S1. Schematic of the multi classification machine learning architecture.

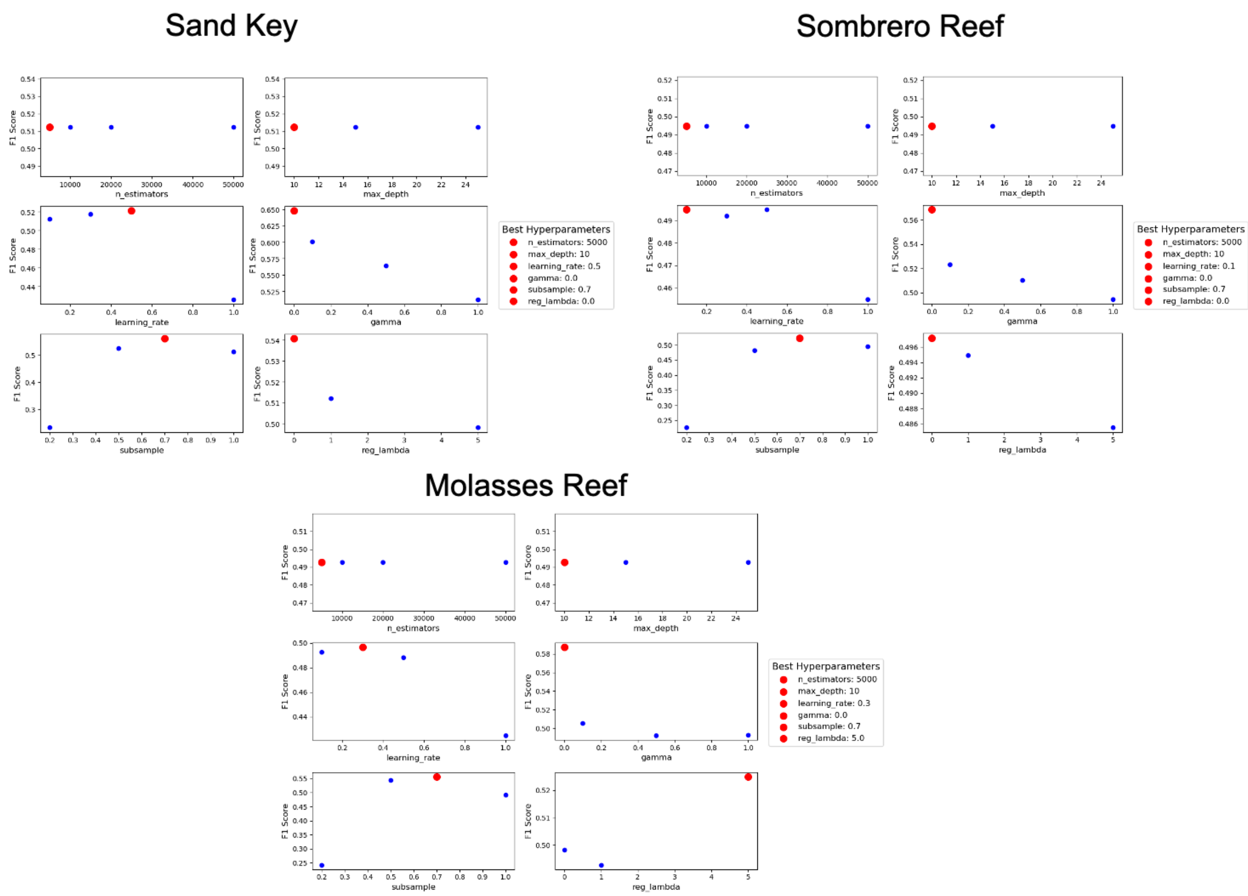

Figure S2. Hyperparameter sweep for each reef site. All hyperparameters are held at the values in Table S2 except for the parameter being assessed. The parameter that results in the highest F1 score is shown in red. Since n_estimators resulted in nearly the same F1 score for all models, we use 20,000 estimators for each model.

Figure S3. Prediction performance for all predictions for the XGBoosted Random Forest model (pink), the Logistic Regression model (gray) and the Frequency Baseline model (green) for the three reef sites for 0-week tolerance. The bar plots show the F1 score (a), onset accuracy (b), no onset accuracy (c), false alarm rate (d) and missed onset rate (e).

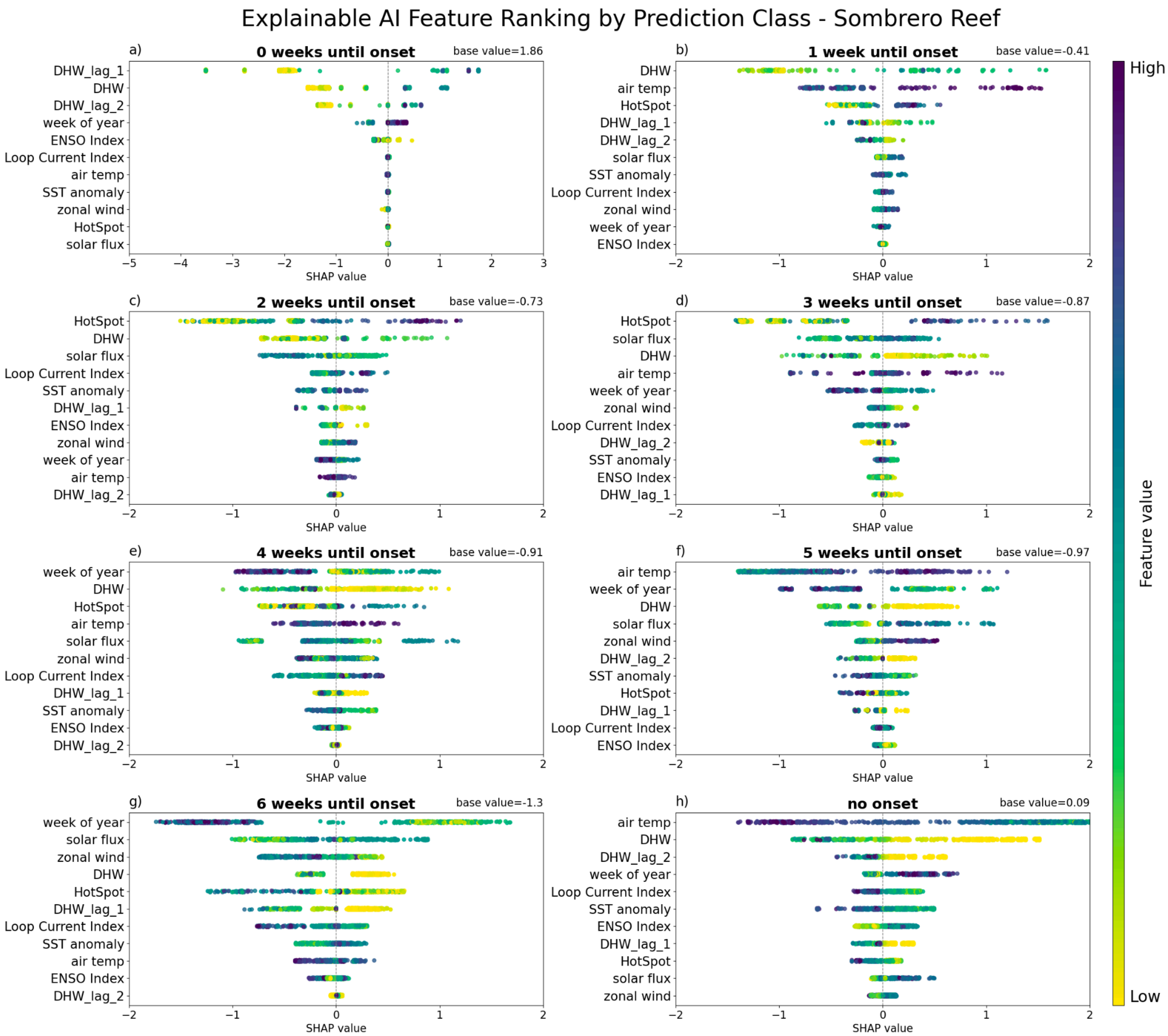

Figure S4. Shapley additive values for test years from all folds using k-fold cross validation (1985-2024) for Sombrero Reef for each prediction class (a-h). The top predictor ranks as most important to the prediction and the bottom predictor is the least important. Purple values indicate higher magnitude of the variable and yellow colors indicate lower magnitude values. Dots with positive SHAP values indicate the predictor increased the probability of that class being predicted, while negative SHAP values indicate the predictor decreased the probability of that class being predicted. The base value, or expected value, for each class is the average model output for that class across all training data.

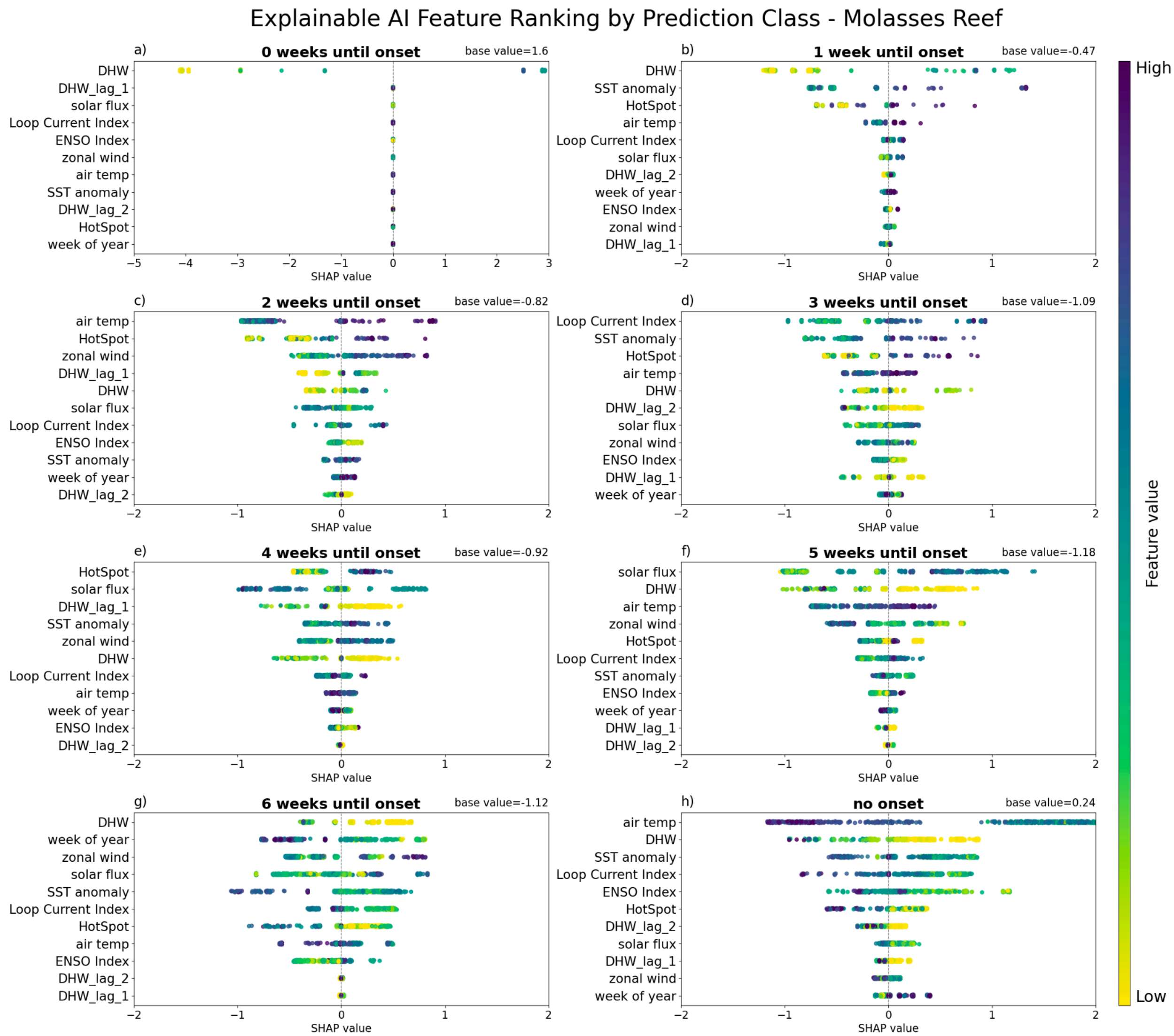

Figure S5. Same as Fig. S4 for Molasses Reef.

Fold	Training Period	Testing Period
Fold 1	1993-2024	1985-1992
Fold 2	1985-1992; 2001-2024	1993-2000
Fold 3	1985-2000; 2009-2024	2001-2008
Fold 4	1985-2008; 2017-2024	2009-2016
Fold 5	1985-2016	2017-2024

Table S1. Training and testing splits for the k-fold cross validation.

Standard deviation of weekly DHW
Standard deviation of SST
Standard deviation of SST anomaly
Standard deviation of HotSpot
500mb geopotential height
925mb meridional wind
Velocity Potential MJO Index PC 1, 2
HotSpot lagged by 1-2 weeks

Table S2. Unused predictor variables. The Velocity Potential MJO Index was obtained from https://psl.noaa.gov/mjo/mjoindex/vpm.1x.txt. All other data taken from the NOAA Coral Reef Watch website or provided by NOAA PSL as stated in the open research statement.

Hyperparameter	**Sand Key**	**Sombrero Reef**	**Molasses Reef**
# of estimators	20000	20000	20000
Max depth	10	10	10
Learning rate	0.5	0.1	0.3
Gamma	0.0	0.0	0.0
Subsample	0.7	0.7	0.7
Lambda regularization	0.0	0.0	5.0
Alpha regularization	1.0	1.0	1.0
Loss (objective)	Softmax	Softmax	Softmax

Table S3. Hyperparameter selection for each reef site.

Sand Key

Model	Correct Onset	Missed Onset	False Alarm	True No Onset	Precision	Recall	F1 Score
XGB	129/220	91/220	192/580	388/580	0.402	0.586	0.477
Linear	27/220	193/220	40/580	540/580	0.403	0.123	0.188
Frequency	170/220	50/220	580/580	0/580	0.227	0.773	0.351

Sombrero Reef

Model	Correct Onset	Missed Onset	False Alarm	True No Onset	Precision	Recall	F1 Score
XGB	115/200	85/200	214/600	386/600	0.350	0.575	0.435
Linear	22/200	178/200	63/600	537/600	0.259	0.110	0.154
Frequency	161/200	39/200	600/600	0/600	0.212	0.805	0.335

Molasses Reef

Model	Correct Onset	Missed Onset	False Alarm	True No Onset	Precision	Recall	F1 Score
XGB	50/120	70/120	230/680	450/680	0.179	0.417	0.250
Linear	20/120	100/120	21/680	659/680	0.488	0.167	0.248
Frequency	78/120	42/120	680/680	0/680	0.103	0.650	0.178

Table S4. Metrics for bar charts in Figure 2 for a tolerance of 1 week.

Sand Key

Model	Correct Onset	Missed Onset	False Alarm	True No Onset	Precision	Recall	F1 Score
XGB	28/77	49/77	71/650	579/650	0.283	0.364	0.318
Linear	30/77	47/77	248/650	402/650	0.108	0.390	0.169
Frequency	2/77	75/77	129/650	521/650	0.015	0.026	0.019

Sombrero Reef

Model	Correct Onset	Missed Onset	False Alarm	True No Onset	Precision	Recall	F1 Score
XGB	34/70	36/70	105/667	562/667	0.245	0.486	0.325
Linear	27/70	43/70	274/667	393/667	0.090	0.386	0.146
Frequency	2/70	68/70	108/667	559/667	0.018	0.029	0.022

Molasses Reef

Model	Correct Onset	Missed Onset	False Alarm	True No Onset	Precision	Recall	F1 Score
XGB	14/42	28/42	47/724	677/724	0.230	0.333	0.272
Linear	9/42	33/42	142/724	582/724	0.060	0.214	0.093
Frequency	2/42	40/42	58/724	666/724	0.033	0.048	0.039

Table S5. Metrics for bar charts in Figure S3 for a tolerance of 0 weeks.