Project Report (FWRI Grant #5473):

Florida's Coral Reef Water Quality Data Compilation, Analysis, and Decision Support
Year 2

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July 1st, 2021 - June 3rd, 2022	$78,356

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Table of Contents

Summary Recommendations

- Combining data without scaling factors is acceptable if the water quality monitoring program uses a NELAC certified lab. Using a NELAC certified lab allows data to be combined across programs without having to account for stoichiometric corrections or differing lab protocols.
- When possible, sampling from different programs should be compared directly from the exact same date, time, and location to test NELAC lab compatibility assumptions, but this is currently unavailable because complete spatio-temporal overlap between any two pairs of programs does not exist in any single location in South Florida.
- Water monitoring programs should consistently report their Minimum Detection Limits (MDLs), and when combining data, we recommend estimating values below MDLs rather than simply converting data below the MDL to zero.
- The most effective way to compare water quality data between programs is through a trend analysis. However, consistent sampling must occur over 10 years to estimate a meaningful trend. In addition to annual cycles, sampling must span multi-year seasonality from a variety of sources (e.g., the loop current).
- Additional water quality monitoring programs, beyond the five most important programs we identified, could be merged into a synoptic master database if they sampled at least three nutrients, sampled more than 5-years, or maintained active sampling.
- Sampling gaps occur on Florida's Coral Reef primarily in the Marquesas and the northern portions of Florida's Coral Reef.
    - Satellite-derived chlorophyll-a could fill some of these gaps, especially via trend analyses and/or in deep water, as the satellite signal is contaminated by reflectance from the sea floor in shallow areas.
    - While there is no satellite product that measures turbidity directly, there is a satellite proxy for turbidity, but this product is expressed in optical units relevant to color, rather than NTU, which is used for in situ measurements. The magnitude of satellite turbidity proxy observations is also markedly different from in situ measurements, so caution is advised when using these products for direct comparisons or to fill gaps.
- There is substantial geographic sampling overlap on Florida's Coral Reef for some water quality parameters, resulting in duplicative and inefficient sampling effort. Therefore, there are opportunities to distribute the same effort over larger geographic regions without compromising sampling integrity.
- Accounting for inconsistent naming conventions, fields, units, and formatting between water quality monitoring programs takes substantial effort.
    - Units: It would be helpful if all programs reported data in the same units.
        - Chlorophyll-a (µg/L), turbidity (NTU), total nitrogen (mg/L) and total phosphorus (mg/L) are already in the same units across all programs.
        - Nitrate+nitrite, phosphate, ammonium and silicate are reported in mg/L by some and µM by others.

- Datasheet: It would be helpful if all programs reported data in the same format with one common datasheet template.
- Station Names: It would be helpful if all programs reviewed their station names to ensure that all unique stations have uniform names throughout the dataset; Spacing, hyphens, dashes, and underscores should match for all entries at the same station to ensure no 'duplicate' stations.

Relevant Programs

93 water quality monitoring programs in Florida were filtered against five criteria (Figure 1):

1) Sampled within South Florida;
2) Sampled at least four water quality parameters of interest (i.e., Chlorophyll-a, temperature, salinity, nitrate+nitrite (NOx), soluble reactive phosphorus (PO4), silica (Si), turbidity, total nitrogen (TN), and total phosphorus (TP));
3) Contains unique sampling data (i.e., not a derivative dataset from another program, or uploaded to multiple portals);
4) Is still actively sampling;
5) Has at least five years of data.

Five of the 93 programs met all of these criteria (NOAA AOML-Walton Smith South Florida ecosystem restoration cruises (AOML-Walton Smith), the Southeast Environmental Research Center water quality monitoring network (SERC), Miami-Dade County's Department of Environmental Resources Management (DERM); the Broward County water quality monitoring program (Broward County), and DEP's coral ecosystem conservation area water quality assessment program (DEP-ECA)). The complete matrix comparing water quality programs can be found here.

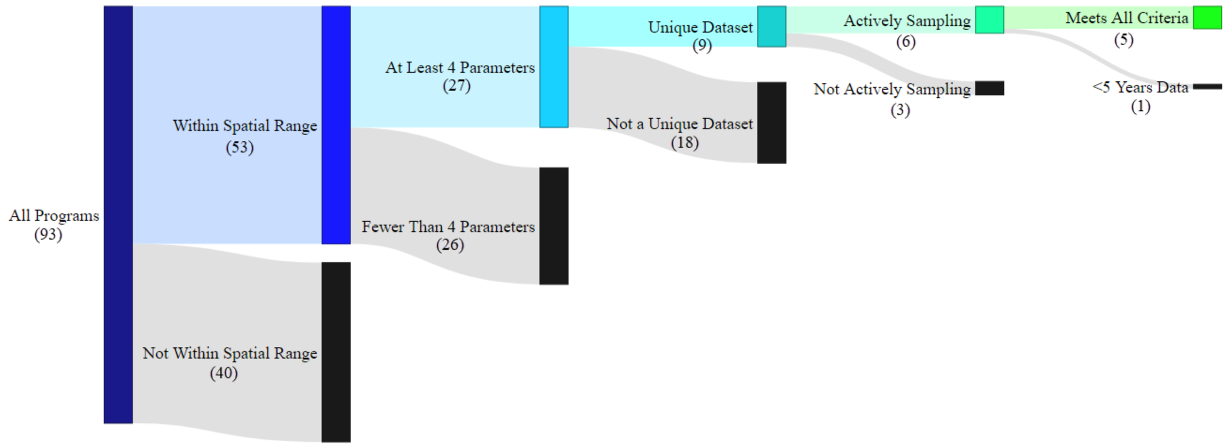

Figure 1. Sankey chart of water quality monitoring programs relevant to South Florida. Five programs met all criteria considered.

Gap Analysis and Geostatistical Findings

The merged programs were analyzed to determine if there were systematic differences in spatio-temporal trends, develop scaling factors to combine data if needed, and identify gaps in sampling. The time series length for each program varies, therefore we examined the trends of each analyte via a seasonal Mann-Kendall test following the methods in Millette et al. 2019, which estimates the Theil-Sen slope as the rate of change in a parameter. The Theil-Sen slope, or rate of change, was used to compare the trends of each parameter of interest across all programs.

The initial comparison of programs was a qualitative examination of spatial trends shown by Theil-Sen slopes in areas of overlap. Theil-Sen slopes were related in areas with high spatial overlap, such as in Biscayne Bay. Therefore, there were no spatial patterns that appeared to yield systematic differences between programs. Rather, divergent rates of change between programs manifested as geographic distance and/or proximity to shore increased.

The qualitative examination was further supported with the quantitative construction of semivariograms for each parameter across the merged dataset. Semivariograms are geostatistical tests that estimate how related samples are depending on the euclidean distance that separates them. Typically, samples closer to each other are more related than samples further apart. Semivariograms are used to model this relationship, and determine the distance, called “range”, at which information from one sample does not provide significant information on the value of another sample. Taking into account this spatial structure can be used to identify if and how samples are highly related (i.e., observe the same process and produce duplicative observations), and potentially allow sampling effort to be combined without compromising observations. For most of the merged parameters, semivariograms demonstrated that sampling could be combined when sampling occurs within specific distances.

Specifically, semivariograms demonstrated variation in the distances at which parameters can be combined, with distances as low as 1.7 km for total phosphorus (TP) and as high as 7.6 km for ammonia (NH4). Total nitrogen (TN) and silicates (Si) semivariograms did not support merging nearby points at any distance, which is likely due to the presence of more complex inshore-offshore trends. TN is largely improving at inland sampling sites, mostly in the southern Everglades and in Broward County, while remaining mostly unchanged offshore. Silicates are not changing across most of Florida's Coral Reef but worsening in southwest Florida. The use of semivariograms to combine TN and Si sampling locations could be improved by splitting the inland from the inshore and offshore locations.

Sampling gaps varied by parameter due to differences in geographic relatedness, as determined by semivariograms, and the number of programs sampling that parameter. Chlorophyll-a was sampled by five important water quality monitoring programs and semivariograms indicated sampling locations could be combined at distances up to 6 km, which results in few sampling gaps across Florida's Coral Reef. Chlorophyll-a sampling is well suited for redistributing sampling effort, especially in areas with high programmatic overlap like Biscayne Bay. Conversely, TP has the smallest geographic range for potential combinations and is sampled by only three programs, resulting in gaps in the northern DEP-ECA and southwest Florida. A few sites in Biscayne Bay can be combined for sampling TP; however, separating inland sites from inshore and offshore locations may broaden the geographic sampling range and allow for the combination of additional sites.

Semivariograms can be used to compute the autocorrelation between samples based on the distance separating sites, or by also considering the relative spatial orientation between each pair of points (e.g. North/South vs West/East). If the only factor affecting autocorrelation is distance, the underlying spatial data are isotropic. However, if the relationship between samples also depends on the relative direction between sites, we need to account for anisotropy in the dataset and appropriately describe the underlying spatial structure in the data (Figure 2). Doing so provides further valuable information for subsequent interpolation methods. Using a non-parametric approximation for the 95 percent confidence interval for the estimated anisotropy ratio parameter (Chorti & Hristopulos, 2008 ; Petrakis & Hristopulos, 2017), we detected potential anisotropy in the merged datasets for chlorophyll-a, ammonium, total nitrogen, and total phosphorus. This can indicate large-scale underlying trends due to systemic structures, dynamics, and processes. Total phosphorus shows that decay in sample similitude (as indicated by higher semivariance) increases more quickly along the WNW/ESE axis, indicating anisotropy in the data. However, when looking at each dataset separately, not all programs were able to detect (or presented) this anisotropic structure, indicating that this phenomenon might also be driven by local environmental and geographic conditions, or that the spatial sampling of some program could not account for this aspect of water quality variation.

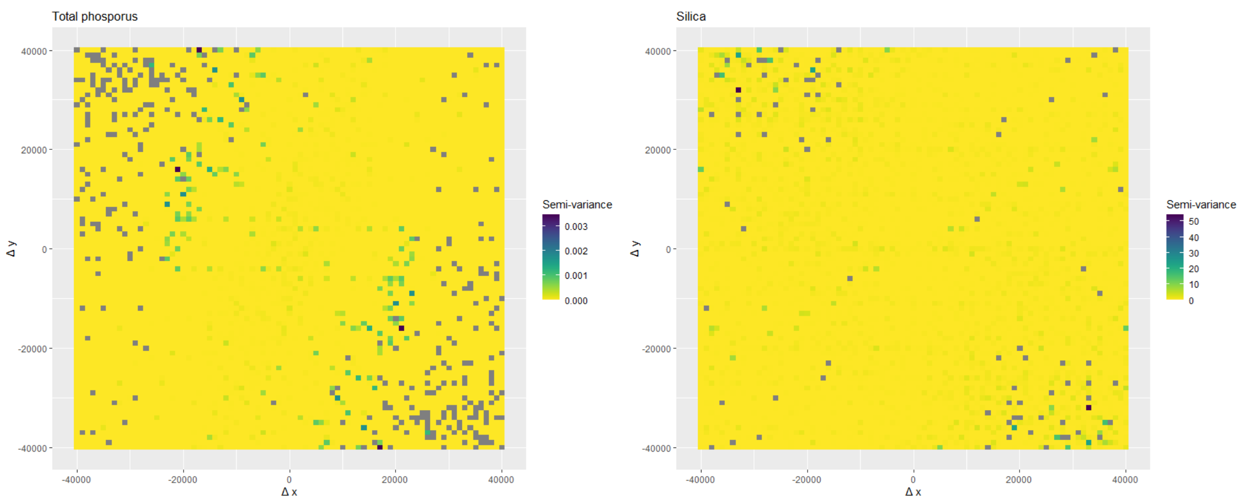

Figure 2. Variogram maps for anisotropic Total Phosphorus (left) and isotropic Silica (right) for merged datasets.

The results from semivariograms can be used to complement point pattern water quality data because semivariograms are the basis for interpolating point pattern data into a continuous prediction (i.e., a raster representation of water quality). We produced kriging surface predictions for all water quality metrics, both for the merged dataset (Figures 3, 4), and each individual program. These maps can be used to estimate the value of a parameter of interest between sampled locations, estimate error due to sampling gaps, and to identify areas of concern or unusual local conditions.

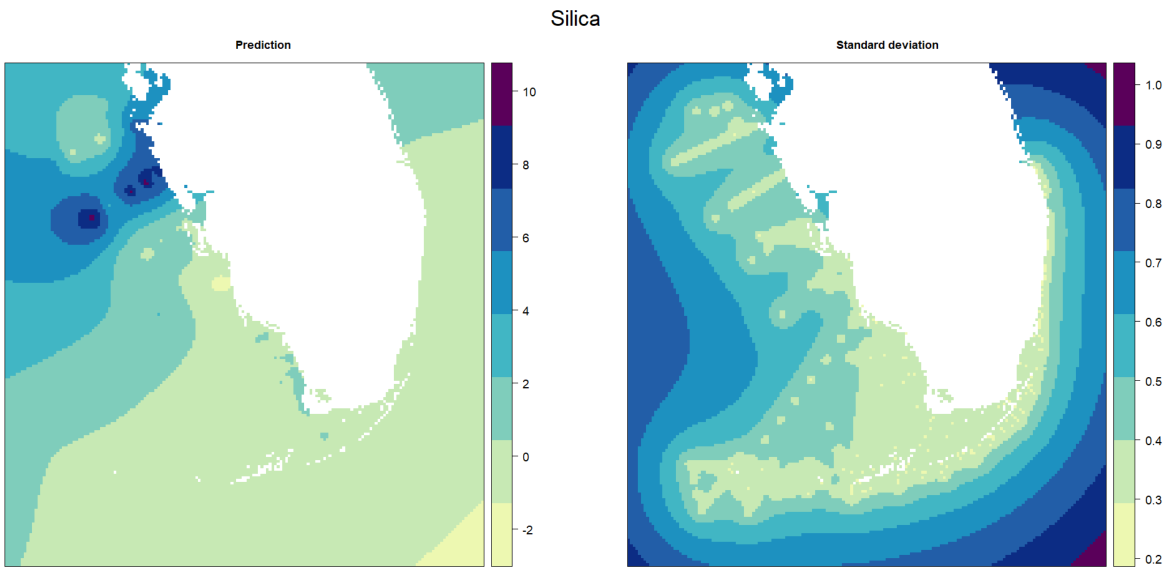

Figure 3. Kriging predictions (left) and associated standard deviation (right) for Silica merged dataset.

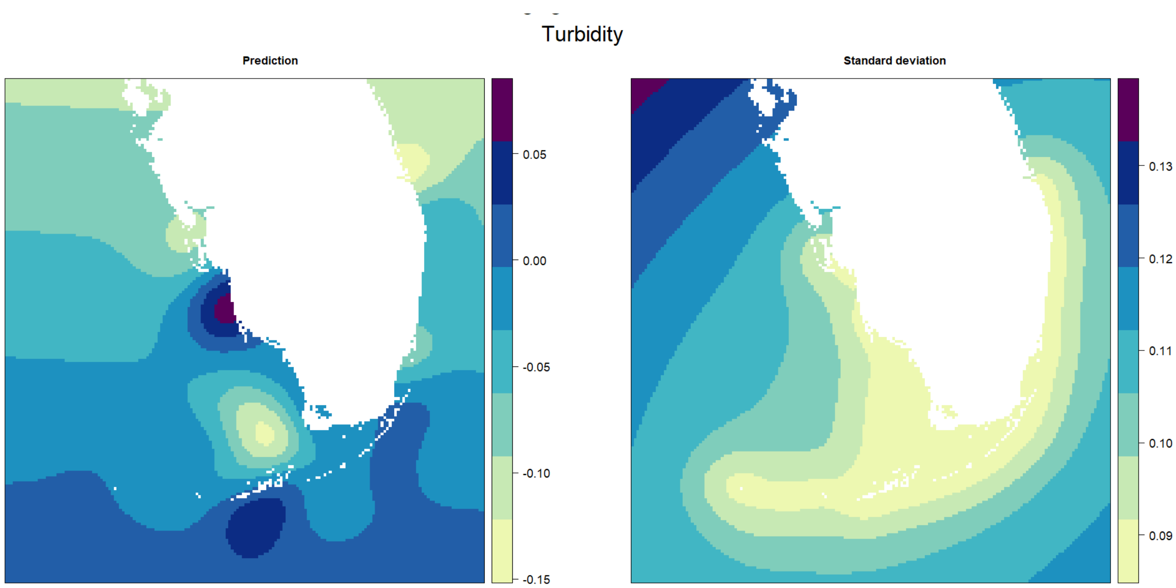

Figure 4. Kriging predictions (left) and associated standard deviation (right) for Turbidity merged dataset.

In addition to estimates of a water quality parameter value in an unsampled area, [kriging interpolation] also produces estimates of the standard deviation. Spatially explicit standard deviation estimates highlight regions that might benefit from increased sampling intensity. Error associated with interpolation, and sampling effort by proxy, is greatest in the Marquesas, the

Dry Tortugas, and the northern reaches of Florida's Coral Reef across all water quality parameters.

Scaling Factors

Five of the most important water quality monitoring programs we identified did not require any scaling factors to be merged together. Each of the monitoring programs used analysis methods approved by the Environmental Protection Agency (EPA) and the labs are all National Environmental Laboratory Accreditation Conference (NELAC) certified. Thus, the results of each parameter should be directly comparable and can be merged without major issues.

The assumption that water quality monitoring programs do not require scaling due to NELAC certification was tested between the Walton Smith and SERC datasets, which overlap regionally. Ten sampling sites from each program located within 1 km of one another, and had sampling periods that overlapped in month and year, were paired together. The time series for the spatially and temporally overlapping sites were compared to test if different methods for the analysis of all four parameters sampled by both programs (NOX, NH4, PO4, and chlorophyll-a) resulted in systematic differences in results. There were no patterns evident to show that either monitoring program was consistently reporting values on a different scale or consistently higher lower value, and thus no scaling factors were identified as necessary (Figure 5). However, the spatial range of these sites, up to 1 km apart, and the broad temporal overlap is a concern. Specifically, sampling dates were aligned by the same month, but analytes can vary daily and hourly with changing tides. When possible, sampling from different programs should be compared directly from the exact same date, time, and location to test NELAC lab compatibility assumptions, but this is currently unavailable because complete spatio-temporal overlap between any two pairs of programs does not exist in any single location in South Florida.

Program specific interpolation methods such as kriging or spatial interpolation by Inverse Path Distance Weighting (Little et al., 1997 ; Stachelek & Madden, 2015) could allow an assessment of the correlation between water quality parameter estimates in overlapping areas and make adjustments to appropriately scale predictions from each program while accounting for the spatial structure underlying each dataset. This could be used to merge estimates and predictions from different datasets as well.

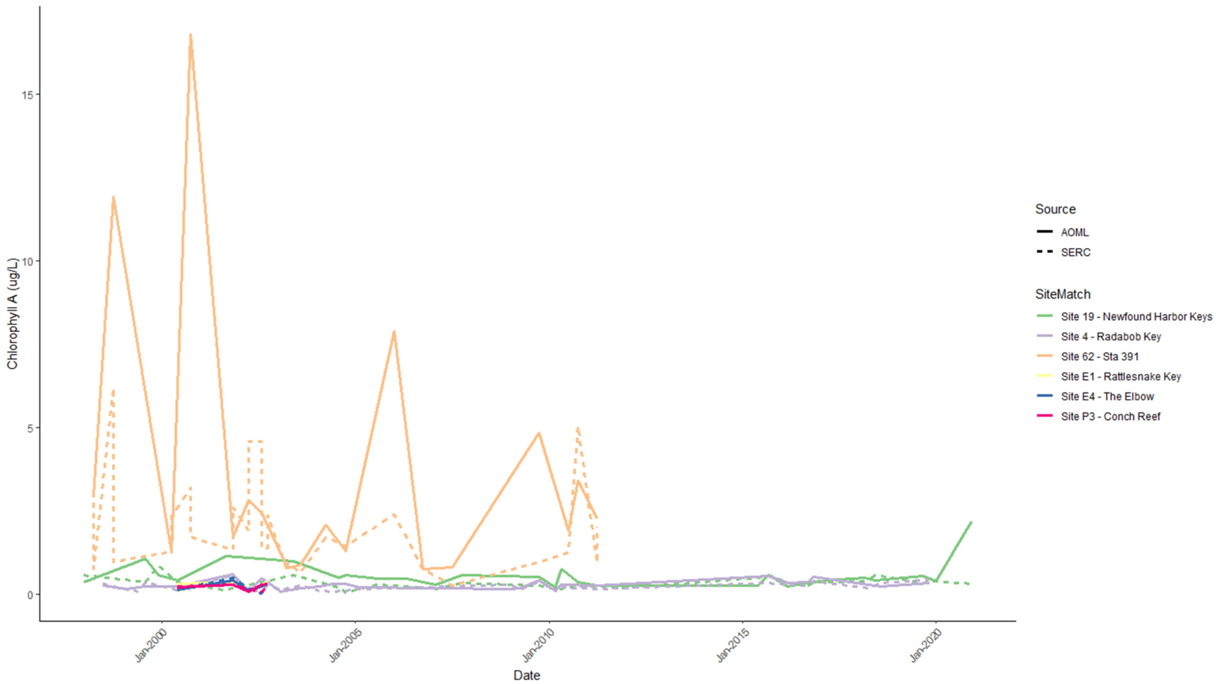

Figure 5. Chlorophyll-a as measured across geographically similar sites between the AOML Walton Smith Cruises (solid lines) and SERC (dotted lines) within the same time period. Comparisons between NOX, NH4, and PO4 exhibited similar relationships.

Minimum Detection Limits

The use of different protocols by monitoring programs, while potentially comparable, results in variation in the minimum detection limits (MDL), or the value below which an analyte cannot be meaningfully measured. Discussions with potential future users of the merged water quality dataset highlighted the importance of handling values below the MDLs. The values below the MDL for each parameter of interest in the merged dataset were estimated using the method described in Flynn et al. 2010. In this approach, the underlying distribution of values *above* the detection limit is used to estimate the values *below* the MDL by minimizing a chi-squared statistic. The Flynn method was applied to the merged data using R code provided by Gareth Williams and Brian Walker. Each water quality protocol has a different MDL, thus applying the Flynn method across the full dataset required the use of a mean MDL, which likely resulted in some values above the detection limit being estimated and some below being left as-is. To avoid this issue, each monitoring program should be encouraged to report MDLs for each analyte and for each analysis protocol. The Flynn method then can be applied within each program and protocol to more accurately estimate values below MDL.

Comparisons between in situ Data and Satellite Products

Direct comparisons between satellite and in situ observations of water quality parameters are not straightforward. The satellite signal is contaminated by bottom reflectance in shallow waters, resulting in satellite observations which are higher than in situ observations because of bottom contamination. Another way to compare satellite and in situ water quality measurements is looking at change over time in a Theil-Sen slope analysis. However, the way Theil-Sen slopes are calculated for satellite and in situ observations is different and introduces a temporal mismatch. Satellite data represent an average over a month, while in situ measurements are at a single point in time. For example, a single in situ measurement at a point in time may capture an event that is averaged out in the satellite data over the month when the in situ data point was measured. It is also important to note that Theil-Sen slopes are highly dependent on the time period used for analysis, so matching the time periods will improve matchups between satellite and in situ slopes.

To assess trends over time and compare with in situ observations, seasonal Mann-Kendall tests and Theil-Sen estimated slopes were calculated based on monthly chlorophyll-a composite images covering the entire West Florida Shelf, using Moderate Resolution Imaging Spectroradiometer-Aqua (MODIS) data from 1/1/2003-12/31/2021. Satellite-derived Theil-Sen slopes were calculated for two products: Chlorophyll-a and remote sensing reflectance at 667 nm (Rrs667), which is a proxy for turbidity. The images in Figures 6 - 9 show chlorophyll-a Theil-Sen slopes for four datasets (AOML-Walton Smith, DEP-ECA, DERM and SERC). Broward County sampling is carried out in canals and in areas very close to shore where satellite observations are not possible. Filled circles overlaid on the satellite image indicate Theil-Sen slopes based on in situ measurements made by NOAA'S Atlantic Oceanographic and Meteorological Laboratory (AOML). The color scales are equivalent for the image and for the circle fill color. Red colors indicate positive change over time and blue colors negative. The units are mg/m^3/year. There is reasonable agreement between satellite and in situ Theil-Sen slopes for chlorophyll-a in Biscayne Bay where negative slopes are seen in each. There is also agreement along the southwest coast of Florida from the mouth of the Shark River north to around Marco Island where mostly positive slopes are observed. Along Florida's Coral Reef, slopes have generally low magnitudes in both satellite and in situ data.

For turbidity or nutrients, there are no satellite products that allow direct comparison with in situ data. There is a satellite proxy for turbidity, but the units do not match in situ turbidity and the magnitudes of the two measurements are markedly different. These two parameters are shown side by side in Figures 10 and 11 with different color scaling to best show the Theil-Sen slopes from the two in situ datasets that include turbidity (DEP-ECA and SERC). For the satellite turbidity proxy, the slopes are generally negative throughout the study area (mean slope = -5.9 x 10^-7) except for a small area south of Cape Sable and a couple of small areas in Biscayne Bay.

This trend is also reflected in the in situ mean Theil-Sen slopes which are negative in both datasets (-0.0173 for SERC and -0.063 for DEP-ECA). Images from figures 6 - 11 can be found here.

In terms of satellite products which are best used for Theil-Sen slope comparisons between satellite and in situ measurements, chlorophyll-a is the best for direct comparison, as the units and magnitudes match for the two measurements. Turbidity is not as straightforward, but can be accomplished by scaling values when comparing slopes from satellite and in situ datasets. We recommend that comparisons with satellite and in situ data focus on Chlorophyll-a and that the time periods used to calculate Theil-Sen slopes be matched.

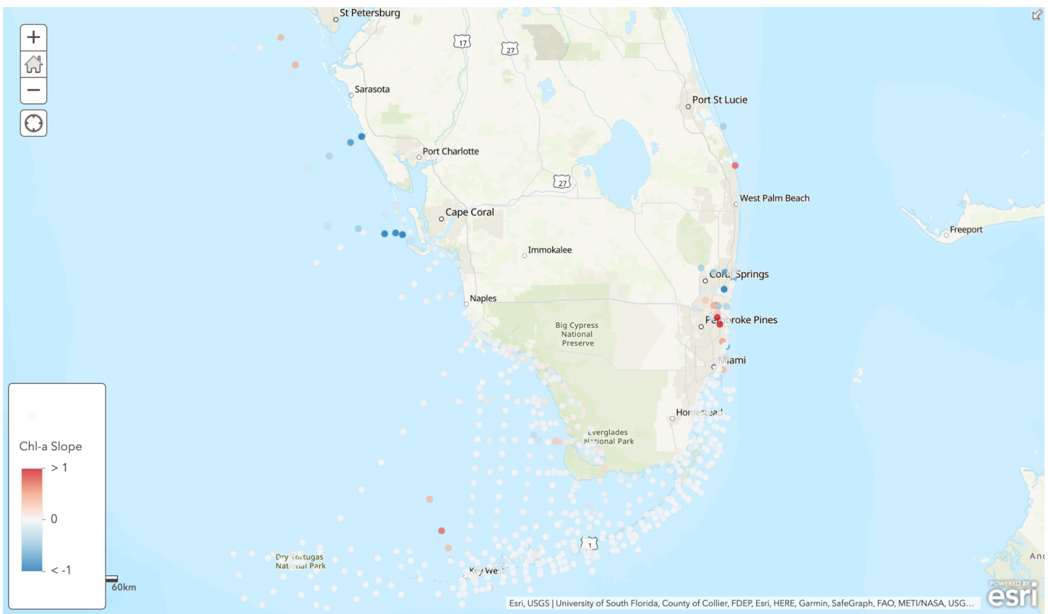

Figure 6. Chlorophyll-a Theil-Sen slope image based on in situ data from all five of the selected water quality programs. Data from 1989-2021 was used to create the image. Red circles indicate an increasing trend in chlorophyll-a concentrations over time, while blue circles indicate a decreasing trend over time. Maps depicting Theil-Sen slopes of other parameters of interest can be found here.

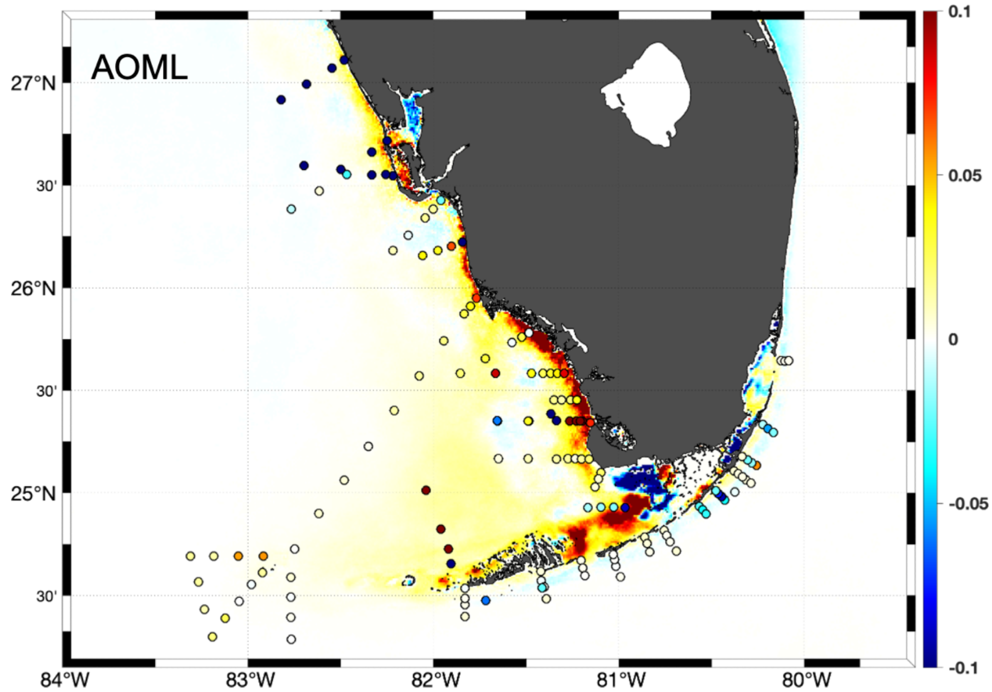

Figure 7. Chlorophyll-a Theil-Sen slope image based on monthly MODIS satellite data (2003-2021). Filled circles indicate locations where in situ chlorophyll-a was measured by NOAA AOML. The circle fill color is based on the same color scale as the satellite image. Units are mg/m^3/year.

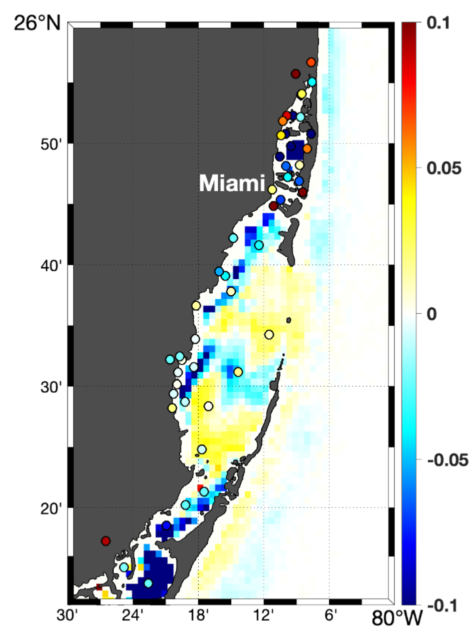

Figure 8. Chlorophyll-a Theil-Sen slope image based on monthly MODIS satellite data (2003-2021). Filled circles indicate locations where in situ chlorophyll-a was measured by the DERM. The circle fill color is based on the same color scale as the satellite image. Units are mg/m^3/year.

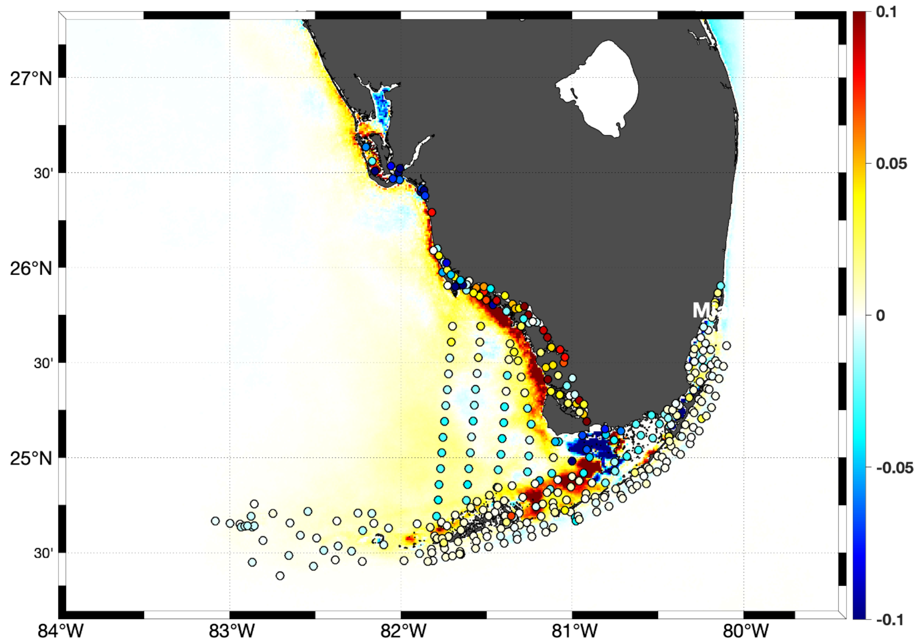

Figure 9. Chlorophyll-a Theil-Sen slope image based on monthly MODIS satellite data (2003-2021). Filled circles indicate locations where in situ chlorophyll-a was measured by SERC. The circle fill color is based on the same color scale as the satellite image. Units are mg/m^3/year.

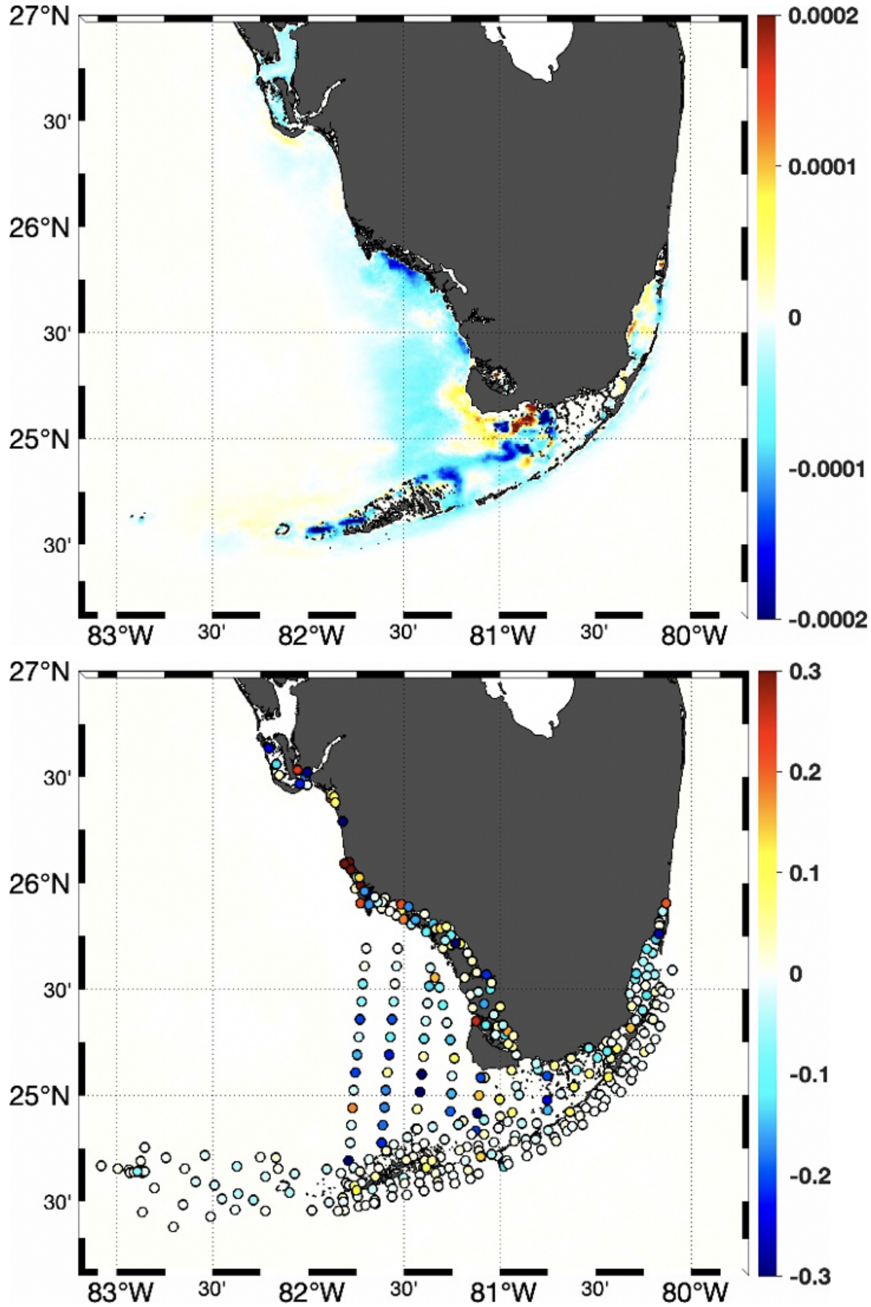

Figure 10. **Top**: Theil-Sen slopes calculated using monthly Rrs667 (a satellite proxy for turbidity) from MODIS satellite data (2003-2021). Units are sr^{-1}/year. **Bottom**: Filled circles indicate locations where in situ turbidity was measured by SERC. The circle fill color is based on the in situ data and is indicated by the bottom color bar. Units are NTU/year.

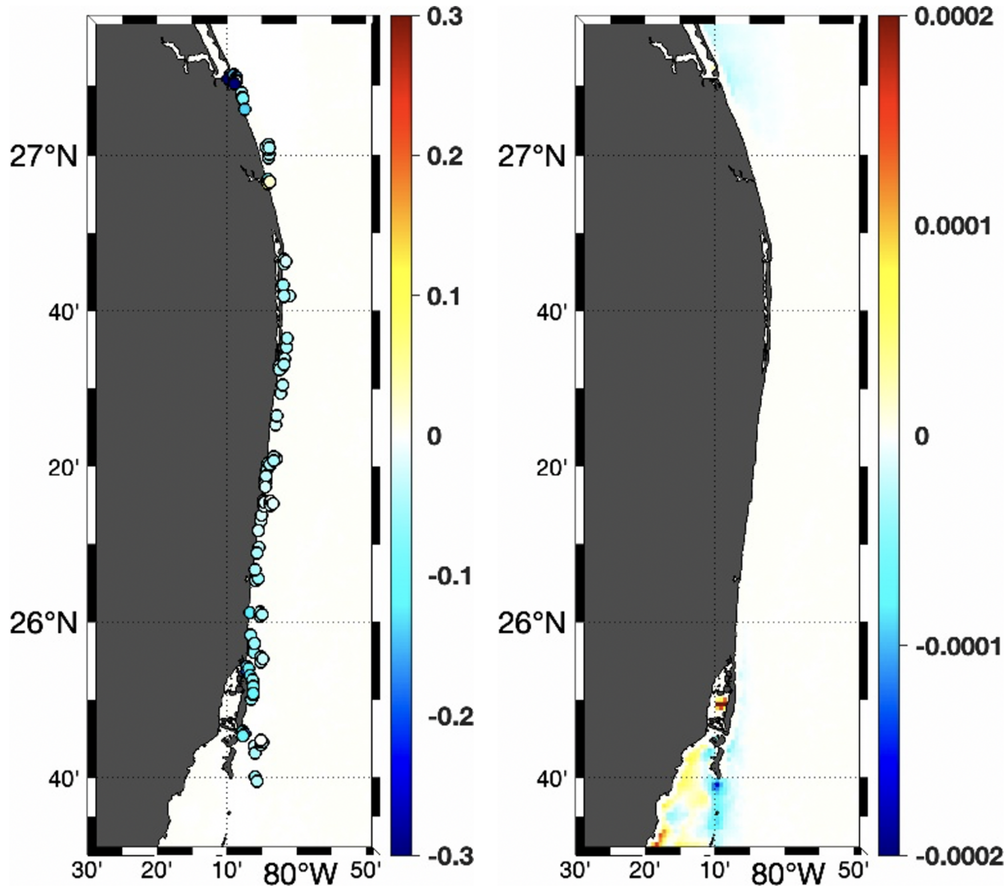

Figure 11. **Left:** Filled circles indicate locations where in situ turbidity was measured by DEP-ECA. The circle fill color is based on the in situ data and is indicated by the color bar at left. Units are NTU/year. **Right:** Theil-Sen slopes calculated using monthly Rrs667 (a satellite proxy for turbidity) from MODIS satellite data (2003-2021). Units are sr^{-1}/year.

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- **DEP-ECA**: Coral Ecosystem Conservation Area Water Quality Assessment
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Selected Meetings, Presentations, and Materials

- October 18, 2021. SEACAR/DEP Water Quality Project Collaboration Meeting.

- November 4, 2021. "Decision Support Tools for Southeast Florida", Southeast Florida Coral Reef Initiative Technical Advisory Committee Meeting.

- January 11, 2022. "Water Quality Programs Associated with Florida's Coral Reef", Department of Environmental Protection. Slides provided to Nick Parr.

- March 25, 2022. "Florida's Coral Reef Water Quality Data Year 2", Department of Environmental Protection.

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