An end-to-end Workflow for Assessing Sea Surface Temperature, Salinity and Water Level Predicted by Coastal Ocean Models

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Abstract— Southeast Coastal Ocean Observing Regional Association (SECOORA) is currently supporting a multi-scale, multi-resolution modeling subsystem for the US Southeast coastal waters to deliver model data and products for coastal resource and emergency response managers and other users. The models that are currently supported in the SECOORA foot print include: regional scale nowcast/forecast ocean circulation modeling system; estuarine and surge/inundation prediction (nowcast/forecast); beach water quality modeling in support of swimming advisories and fisheries habitat modeling for improving stock assessment. Effective use of coastal ocean model forecasts requires a thorough understanding of model skill for different environmental scenarios, regions and times. Computation of model skill, however, has historically been difficult due to varying data conventions, distribution techniques and lack of general tools for discovery, access and use. SECOORA is addressing this problem by developing reproducible workflows for model skill assessment that can be run on any Mac, Windows or Linux computer using free, extensible software. The workflow first discovers datasets via a catalog search over the distributed data holdings of US-IOOS, using bounding box, time range and variable search capabilities of the Open Geospatial Consortium (OGC) Catalog Services for the Web (CSW). The workflow then locates known web service endpoints (OGC Sensor Observation Service (SOS) for sensor data, OPeNDAP with Climate Forecast (CF) Conventions for model output) in the metadata, and extracts data directly from these distributed services. The workflow then extracts time series from the observations and models, does QA/QC, and computes skill metrics in an automated fashion. The results are also displayed qualitatively in an interactive mapping function. The workflow has been written using python within the IPython Notebook (aka Jupyter Notebook), which allows using a standard web browser as a client, and documents the workflow. The environment required to run the notebooks has also been standardized, allowing anyone to install and reproduce our results using free software in a matter of minutes.

Keywords—; Coastal Ocean Observing; Ocean Circulation Model; Skill Metrics; Sensor Observation Service; Metadata; Catalog Services

I. INTRODUCTION

The Southeast Coastal Ocean Observing Regional Association (SECOORA) is one of the eleven coastal ocean observing regional associations established in partnership with the US Integrated Ocean Observing system (US IOOS®). The SECOORA footprint encompasses coastal estuarine and ocean waters of North and South Carolinas, Georgia and Florida. The U.S Southeast (SE) coastal region is vulnerable to hurricane hazards, potential impacts from oil spills, and climate change because of low land elevations, corals and other critical habitats, and our location at the transition of tropical to subtropical latitudes. SECOORA is in the process of implementing an end-to-end regional coastal ocean observing system (RCOOS) that leverages, integrates and augments existing observational, modeling, data management, education and scientific assets within the region. The observing subsystem provides the basis for the RCOOS by supporting and integrating existing assets and observations specific to the timely delivery and development of products. The observing subsystem consists of a suite of coastal and offshore moored platforms, autonomous underwater gliders, satellite data

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receivers and high-frequency radar (HFR) surface current installations. SECOORA follows an optimal approach to advance the implementation of SECOORA models from sub-regional to regional scales, including coupled atmosphere, surface wave, water quality, habitat and ocean circulation models. SECOORA has established a robust data management and communications infrastructure, and has implemented the Integrated Ocean Observing System (IOOS®) Data Management and Communications (DMAC) recommended standards and technologies that promote interoperability, aggregation, access, discovery, visualization, utilization, archival and dissemination of coastal ocean observations and model data. An understanding of model skill is critically important for effective use of ocean forecasts. With multiple models running in different regions of the ocean, we need to understand which models work best in different regions and for addressing different issues (e.g. water levels during storms, waves, surface currents and temperatures for swimmers). This has historically been a task only experts can perform, due to different file conventions, data formats, distribution systems used by the ocean model and observation providers. This results in limited assessment of model skill, usually performed after initial model calibration. Thanks to standardization of web services, freely available tools to access these services, and systems that allow software environments to be freely and easily reproduced, it is now possible to build skill assessment tools that can be run continuously, and freely reproduced by others.

US-IOOS has implemented a model-data discovery and access system in which users can access the data in standardized manner [5]. The system consists of standard web services and conventions like OPeNDAP (Open-source Project for a Network Data Access Protocol) with CF conventions, SOS OGC Web Mapping Service (WMS). ISO metadata [4] is routinely extracted from these services, and harvested into a central, searchable database. This allows all registered US-IOOS observational and model data to be discovered via a single point of access using the Open Geospatial Consortium (OGC) Catalog Service for the Web (CSW). To allow their model products to be used appropriately in addressing regional issues, we are leveraging the US-IOOS data management standards and services and SECOORA DMAC infrastructure to create a free automated open-source skill assessment package that any US-IOOS region can use, and could easily be adapted by other communities in the geosciences.

II. MODEL SKILL ASSESSMENT

A. Data Discovery

The first step in developing the automated on-line Model Skill Assessment tool is the discovery of model and observational data. Datasets are discovered by a catalog search over the distributed U.S. IOOS data holdings, web service endpoints are extracted from metadata, data are then extracted from these web service endpoints, and skill metrics are produced (Figure 1). The automated catalog search incorporated in the model skill assessment workflow facilitates the discovery of new observational and model data that becomes available. We query the US-IOOS CSW endpoint using the OGC Web Service utility library (OWSLib) package, which allows sophisticated queries to be easily constructed.

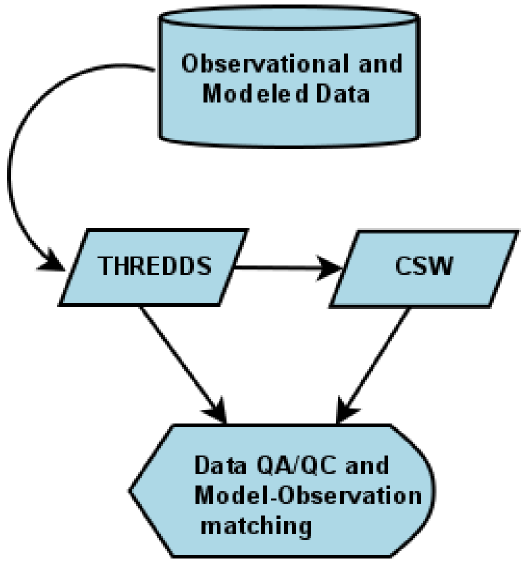

Figure 1: The model data skill assessment workflow. Collections of model output are aggregated and standardized as a single dataset using the THREDDS data server. The harvested metadata from the THREDDS server is searchable via a CSW service. The application first searches for data using CSW, then extracts data from THREDDS using the endpoints it discovered in the metadata returned from the CSW service.

These queries typically include a bounding box (Latitude and Longitude), a date and time range and a certain variable of interest. The query returns records obtained via the CSW, and the IOOS supported service end points are extracted from the metadata. The service endpoints for observational data is the OGC Sensor Observation Service (SOS), and for model output it is OPeNDAP with Climate Forecast (CF) Conventions.

B. Data Access and Use

To access the needed observational data for our model skill assessment work, the IOOS DMAC recommended SOS data access service was used. The SOS provides access to sets of in-situ temperature, salinity, currents, water level, waves and winds data in the CSV, TSV, XML and or KML format. We access the time series of Sea Surface Temperature (SST), Sea Surface Salinity (SSS) and Sea Surface Height (SSH) observations in the SECOORA region collected by academic, state and federal agencies. For accessing the model data, we utilize the Iris package [3] which leverages the CF Conventions. The package returns geospatial and temporal coordinates associated with data from any CF-1.6 compliant model result. The model data that we identified via search for use for this study are: USGS Coupled Ocean Atmosphere Wave Sediment-Transport (COAWST) Forecast System; Rutgers University Experimental System for Predicting Shelf and Slope Optics (ESPreSSO); HYbrid Coordinate Ocean Model (HYCOM); North Carolina State University (NCSU) South Atlantic Bight and Gulf of Mexico (SABGOM)

Nowcast/Forecast System and US East Nowacst/Forecast system; University of South Florida Finite-Volume, primitive equation Community Ocean Model (FVCOM) and Regional Ocean Modeling System (ROMS).We extract the time series of data from the model grid point nearest to the available observational data. This is more challenging, because depending on the model, the horizontal coordinate of the output data may be on a regular, curvilinear, or unstructured (e.g. triangular) grid, while the vertical coordinates may be on a uniform or non-dimensional grid with a number of different possibilities (e.g., sigma, s-coordinate, isopycnal, etc). The data are then run through a simple Quality Assurance and Quality Control (QA/QC) routine, and a week worth of a station time series is stored. The QA/QC consists of spikes removal and rudimentary gross range test. The time series of both observational and model data are saved in 30 minutes interval every week and displayed in the interactive map allowing qualitative comparison of time series plots (Figure 3 and Figure 4). We open the datasets using the OPeNDAP URL, identify the model grid cell nearest to the observational location. If the model grid cell is within a specified distance (5 km) from the sensor location, time series data is extracted. Because the temporal time differences on the availability of model and in-situ observations (e.g., hourly or fifteen minute etc.) and model data (e.g. once every three hours etc.), we interpolate them onto a common time base (3 hours).

III. Model skill Assessment

Once we have the quality controlled time series of observational and model data, we then compute model skill metrics. Following [7], the skill metrics computed are the Model Bias (MB), Centered Root Mean Square Error (CRMSE), and Cross Correlation (R2) and results presented in Table 1 and 2. We compute these skill metrics on a weekly basis. In this work, we are presenting the preliminary results of the automated model skill assessment tool and associated output products. The variables we assessed were Sea Surface Temperature (SST), Sea Surface Salinity (SSS), and Sea Surface Height (SSH) time-series. Model skill may be low because of high noise in the data, or it may artificially high due to correlated properties in the model and data, e.g. tides for example [2]. To avoid extreme events like storm surges, we computed the skills twice: first against the original series, then again using a low-pass 40 hours Lanczos filter to remove the tides [1] Only the filtered skill score is reported in the interactive map because most coastal ocean models are quite skillful to predict tides due to the use of independent tidal harmonic as boundary conditions.

We present here the results of comparison for a single week from 2015-07-31 to 2015-08-07. A CRMSE of 1 means perfect a perfect fit, zero means the model has no skill, and negative values means the model has no more value than the mean itself. The CRMSE does not account for the model Mean Bias (MB). The largest MB is observed in the HYCOM Model, which is not surprising since this is a global model (Table 1). The second largest bias is found in the SABGOM model. The computation and interpretation/verification of the results presented are yet to be carried out with the modeling group/scientists.

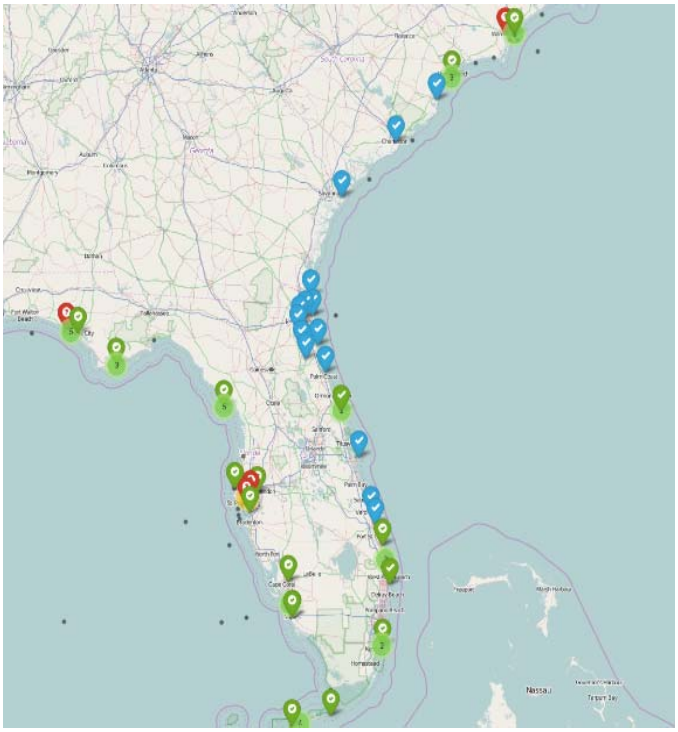

Figure 3. Interactive map showing all the observations in SECOORA region via CSW search. The colored coded icons are green for where model and observations are found, blue for observations only, and red for observations that cannot be used in the comparison because of data elevation issues of the observational data.

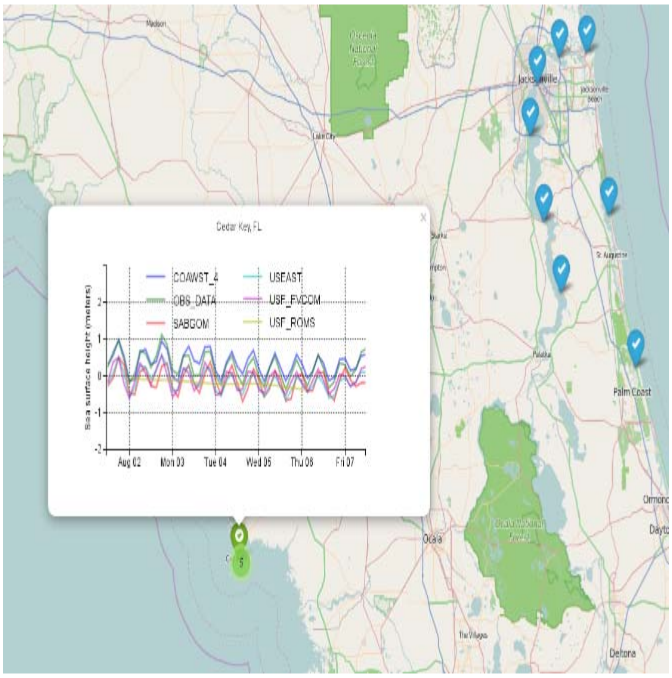

Figure 4: Interactive map popup showing the water level data (model and observation) comparison for Cedar Key, FL

In-situ Station	COA WST	ESPRE SSO	HY COM	SAB GOM	US EAST	USF FVCOM	USF ROMS
Duck, NC				0.47			
Oregon Inlet Marina, NC	0.29	0.60	0.91				
Wrightsville Beach, NC	0.13		0.98	0.56			
Springmaid Pier, SC	0.14			0.58	0.51		
Lake Worth Pier, FL	0.45						
Virginia Key, FL				0.26	0.14		
Vaca Key, FL						0.18	
Key West, FL	0.35			0.16		0.11	
Naples, FL						0.17	0.16
Fort Myers, FL						0.22	0.31
Port Manatee, FL						0.24	0.15
Mckay Bay Entrance, FL						0.31	0.28
Clearwater Beach, FL						0.46	0.09
Cedar Key, FL	0.15			0.40	0.40	0.36	0.26
Apalachicola, FL	0.09					0.36	0.38
Panama City, FL	0.07						0.29
Pensacola, FL	0.06						
Naples Bay station						0.20	0.13
Ponce De Leon South station	0.21		0.48				
St Lucie Inlet station	0.37			0.16			
Average Skill	0.21	0.60	0.79	0.37	0.35	0.26	0.23

Table 1: Example Sea Surface Height model bias (MB) at each observed station, computed for the week 2015-07-31 to 2015-08-07. These metrics are computed for each week, so that skill during different type of forcing conditions may be analyzed. output outside the barrier, as long as the distance criteria is met. These special situations highlight the need for careful examination of the results, and likely need for invocation of custom filters depending on the goals of the particular skill assessment.

In-situ station	COAW ST_4	ESPRE SSO	HY COM	SAB GOM	US EAST	USF FVCOM	USF ROMS
Duck, NC				0.41			
Oregon Inlet Marina, NC	-7.73	-4.58	-3.83				
Wrightsville Beach, NC	-1.57		-0.67	0.00			
Springmaid Pier, SC	0.27			0.46	0.44		
Lake Worth Pier, FL	-1.48						
Virginia Key, FL				-0.38	-0.32		
Vaca Key, FL						0.10	
Key West, FL	0.46			-0.47		0.23	
Naples, FL						0.74	-1.27
Fort Myers, FL						0.60	
Port Manatee, FL						0.76	
Mckay Bay Entrance, FL						0.73	0.82
Clearwater Beach, FL						-0.10	0.45
Cedar Key, FL	0.69			0.65	0.96	0.68	0.61
Apalachicola, FL	0.56					0.85	-1.33
Panama City, FL	0.59						
Pensacola, FL	0.49						
Naples Bay station						0.78	-13.38
Ponce De Leon South station	-2.17		-4.75				
St Lucie Inlet station	-1.70			0.76			
Average Skill	-1.05	-4.58	-3.08	0.20	0.36	0.54	-2.35

Table 2: Sea Surface Height model skill (CRMSE) for the tidal filtered series at each observed station, computed for the week 2015-07-31 to 2015-08-07. These metrics are computed for each week, so that skill during different type of forcing conditions may be analyzed.

A. Reproducibility

Reproducibility is a cornerstone of science, and reproducing scientific data analysis requires open and standardized access to the data, tools that can search, access, analyze and visualize the data, and a software environment that allows tools to run regardless of computing platform. US-IOOS has addressed the access issue by requiring data providers to provide standardized data services, and we have addressed the tools issue by creating reproducible IPython/Jupyter notebooks (Figure 5) that demonstrate the use of standardized tools to compute the skill assessment metrics. For the software environment issue, there are several challenges: installing the required software; providing a consistent environment for all platforms (Windows, OS X, Linux); ensuring the software versions match and are compiled in a consistent way against their dependencies. To address these issues we created a repository (or channel) for software binaries using the Open Source package and language-agnostic Conda packager. The binaries are built via a "recipe" and GitHub is used to keep the recipes under version control. The use of GitHub allows any user to send recipes updates or improvement as well as manage issues and suggestions to the software stack hosted in the channel.

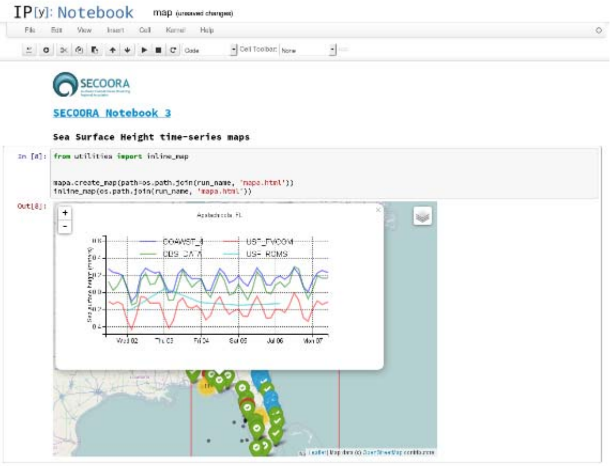

Figure 5. Screenshot of a skill-assessment IPython/Jupyter reproducible notebook. The SECOORA skill assessment workflow is completed with three sequential notebooks: the 1st notebook finds and extracts data, the 2nd computes skill metrics, and the 3rd creates plots.

Continued Integration (CI) services are used to build and upload these binaries to the channel. The CIs used are: Circle-CI (Linux-32/64), Travis-CI (OS X-64), and AppVeyor Windows-32/64). All these services start automatically, via GitHub hooks, every-time a recipe is modified. However, the binary is only uploaded to the channel when the recipe change is merged into the repository. This workflow grants the opportunity for tests and quality control of the software that is uploaded to the channel. The result is reproducibility: within 15 minutes, anyone on Mac, Linux or Windows can download and install a free computing environment that will run our skill assessment notebooks. Not only can they reproduce them, but they can adapt them for their own purposes, or use them as a launch point for entirely new investigations.

IV. CONCLUSIONS

We have developed a flexible, standardized, reproducible set of scientific notebooks for model skill assessment. These notebooks were applied here to temperature, salinity and water level data, and work is being carried out to evaluate and compare horizontal and vertical slices using satellite, CTD, and glider data. In addition, although they were applied here in the SECOORA region, they could be applied in any region by just changing the bounding box. We hope that by providing reproducible skill assessment notebooks, the results will not only be verified, but will be expanded to test new aspects of model skill, and applied to more models in more regions. When the model skill is known, it can then be used by modelers to investigate and improve their models, and also used by model data consumers to determine appropriate use of the models. This results in better models and more effective use of model results.

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