Supporting Information for "Estimating historical air-sea CO$_2$ fluxes: Incorporating physical knowledge within a data-only approach"

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Contents of this file

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S1. Large Ensemble Testbed Findings

Utilizing the Large Ensemble Testbed (Gloege, McKinley, et al., 2021), we analyzed how RMSE was impacted by reconstructing the pCO_2-Residual instead of pCO_2. The Large Ensemble Testbed consists of 25 ensemble members each from 4 Earth System Models. Within this model setting, we sample model features and pCO_2 at the same times and locations as we have actual SOCAT observations, in every ensemble member. Just as done with actual observations, an XGBoost algorithm is trained on the subset of features and pCO_2 from the models. We then reconstruct pCO_2 everywhere using the resulting functions and compare the reconstructed pCO_2 to the model "truth". Thus, the reconstructed pCO_2 can be evaluated at all times and locations simulated within the models, not just where we have SOCAT observations. Figure S1 shows that in addition to reducing the RMSE of the test data for each reconstruction ("test data"), RMSE across the globe, where the model has never been sampled ("unseen data"), is reduced using the pCO_2-Residual approach. Note also that against both test and unseen data, the high extreme RMSE is reduced by at least 3 μatm.

S2. Uncertainty Due to Chlorophyll Climatology

Within the Large Ensemble Testbed, we use XGBoost to reconstruct pCO_2 using time-varying chlorophyll-a (every month has modeled chlorophyll-a) and compare to when the monthly climatology of model chlorophyll (1998 onward) is used for prior to 1998. As we do not have satellite observations of chlorophyll-a prior to 1997, this techniques estimates uncertainties caused by using a climatology of chlorophyll-a for the years prior to satellite observations. The calculated air-sea CO_2 flux differs significantly prior to the mid-1990s

and decreases to approximately 0.05 PgC/yr by 2005. There is variation across the models, with the largest mean impact on the reconstruction seen within the MPI model. The mean difference across the ESMs and time is less than 0.1 PgC/yr.

S3. RMSE, Bias, MAE in pCO$_2$-Residual approach

The map of mean RMSE against all SOCAT observations using the pCO$_2$-Residual algorithm is shown in Figure S3. We see lowest RMSE in temperature-controlled regions, with values less than 10 μatm, as expected, and higher RMSE outside of these regions.

S4. Test of Clustering with Self-Organizing Maps

To examine whether the regression would be improved by dividing the global ocean into biomes, we utilized the self-organizing map package SOMPY (Moosavi et al., 2014) (https://github. com/sevamoo/SOMPY). The global ocean was divided into 5, 10, and 15 clusters using maximum annual ice fraction, mean pCO$_2$, mean annual sea surface temperature, mixed layer depth, and spring mean chlorophyll (Fay & McKinley, 2014). On the global scale, there was no added skill, quantified based on RMSE and comparisons to independent data at BATS, HOT, LDEO, or GLODAP. We therefore maintain the simpler model.

References

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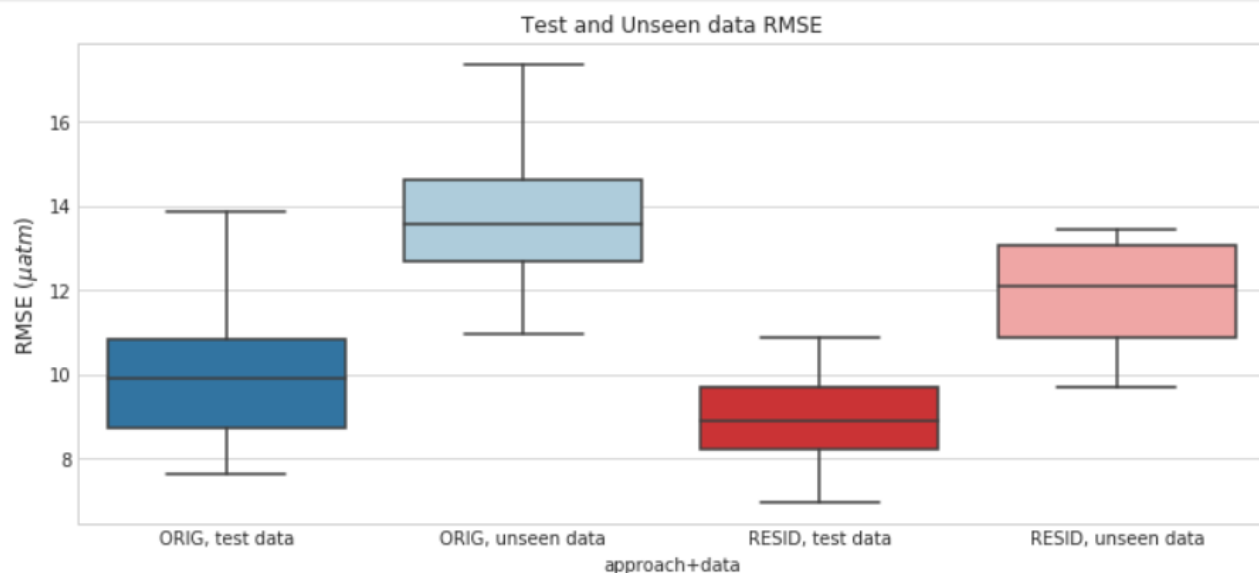
Figure S1. Test RMSE for pCO_2 reconstruction (ORIG, test data); RMSE at locations not sampled by SOCAT for pCO_2 reconstruction (ORIG, unseen data); Test RMSE for pCO_2-Residual approach (RESID, test data); RMSE at locations not sampled for pCO_2-Residual approach (RESID, unseen data). Each boxplot contains the 100 ensemble members, 25 from each Earth System Model of the Large Ensemble Testbed (Gloege, Yan, et al., 2021).
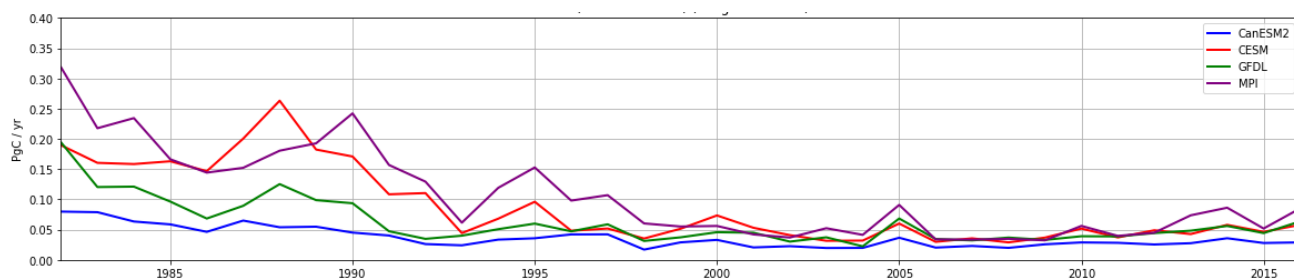

Figure S2. Absolute value of difference in globally-integrated reconstructed CO_2 flux (PgC/yr) when using a climatology of chlorophyll-a prior to 1998. Different colors represent the four different ESMs.
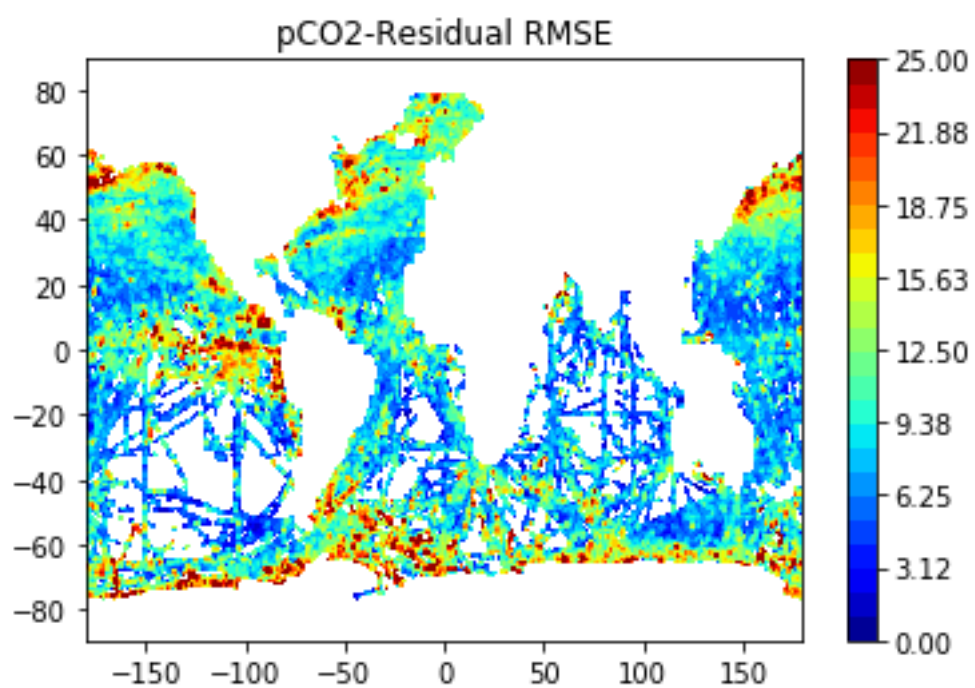
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Figure S3. Mean RMSE (μatm) across the global ocean using the pCO$_2$-Residual approach.