Review of bg-2017-64 “Global high-resolution monthly pCO2 climatology for the coastal ocean derived from neural network interpolation” by Laruelle et al.

This manuscript proposed a modified two-step artificial neural network method for deriving pCO2 (SOM-FFN, Landschützer et al., 2013), and focused on shelf seas. The most important modification are (1) much higher resolution as 0.25 degree; (2) inclusion of sea-ice as a predictor of pCO2. From this effort, the authors may present a fine scale coastal sea pCO2 globally, as Fig. 2 in the manuscript shown. This is certainly of value. However, there are some major issues. The method is not new, rather an interpolation of the open ocean model.

We are pleased to see that the reviewer values our coastal pCO_2 maps and are grateful for his constructive remarks and suggestions. We understand that the reviewer is not fully convinced by the novelty of the method and the added value our manuscript under its current form. As explained in answers, we do not concur with the statement that our model only is an extension or interpolation of the previously existing oceanic model. Instead, we believe that it is a significantly modified version, specifically tailored to reconstruct the complex coastal pCO_2 cycle. In the updated manuscript, we propose to put more emphasis on the modifications of the original SOM_FFN and compare our coastal set up with the open ocean one. Further attention will also be given to better quantifying the improvements resulting from the modification of the open ocean set-up from Landschützer et al. (2013) and identifying the remaining knowledge gaps (see also replies to comments 2, 7, 14 of reviewer 1).
The reviewer was also concerned by the weakness of the validation of our results performed using a database that largely overlaps with the database used to calibrate the model. Following both reviewer’s recommendations, we modified our approach and, using the latest versions of both SOCAT (i.e. version 4) and LDEO (i.e. v2015), we created two entirely independent datasets, named SOCAT* for the calibration and LDEO* for the validation. These two datasets were generated by randomly assigning each measurement common to both original databases to either SOCAT* or LDEO* (see comment 2 below for further details on the new approach). In addition, we have also introduced a new predictor (wind speed), which helped improve the performances of the SOM_FFN compared to those presented in the previous version of the manuscript.
Please find bellow a detailed answer to each comment. All our answers are written in blue and the modifications within the text are highlighted in bold and italic.
On behalf of all co-authors,

Goulven Laruelle

It was said that all data were converted to 0.25 degree from their original resolution. Then please indicate clearly original resolution of each data, for example, SSS, SST and depth. At least for SST and SSS from the World Ocean Atlas, I wonder if the resolution is fine in the shelf seas (sorry I do not
check, my memory is 1 degree). If it is true, I do not think such an interpolation of SST and SSS would help in deriving really high resolution pCO2 (i.e. the final result might be close to a simple interpolation of modeling pCO2 of 1 degree resolution).

[1] The spatial resolution of SST and SSS from the World Ocean Atlas is indeed only 1 degree. In response to the reviewer’s comment, we now apply 0.25° resolution datasets

for SSS and SST by using Met Office's EN4: quality controlled subsurface ocean temperature and salinity profiles and objective analyses (Good et al., 2009). By doing so, all predictors used for the calculation of the SOM_FFN have now resolution of 0.25° or higher. We also propose the inclusion of the table below, which lists the selected datasets used, their purpose (i.e. calibration, validation…) and original spatio-temporal resolution.

We reiterate here that we disagree with the notion that our model is a mere interpolation of the global oceanic model developed by Landschützer et al. (2013). Although both the coastal SOM_FFN presented in this study and the oceanic SOM_FFN published in Landschützer et al. (2013) share common methodologies, they were not trained with the same datasets. For the most part, the coastal data from SOCAT used here for calibration and validation was not included in the data pool used for the open ocean simulations. In addition, the ranges of values (within which both models are trained) are also different for some of the environmental parameters. In particular, the average bathymetry and sea surface salinities are often significantly lower in coastal regions than in the open ocean. We thus believe that the important physical and biogeochemical differences between coastal and open oceanic waters fully justify careful retraining of the SOM_FFN. In addition, the typical spatial scales of physical and biogeochemical gradients in nearshore waters are often smaller than 1 degree and justify the implementation of the SOM_FFN at a higher resolution. Nevertheless, to better demonstrate the value of our approach, we follow the comment of the reviewer and discuss in more details the comparison between open and coastal ocean models in the revised manuscript.

Table 1: Datasets used to create the environmental forcing files. The original spatial and temporal resolution and the main manipulations applied for their use in the SOM_FFN are also reported.

Predictor	**dataset**	**resolution**	**reference**	**Manipulation**
SST	EN4	0.25°, daily	Good et al., 2013	Monthly average
SSS	EN4	0.25°, daily	Good et al., 2013	Monthly average
Bathymetry	ETOPO2	2 minutes	US Department of Commerce, 2006	Aggregation to 0.25°
Sea ice	NSIDC	0.25°, daily	Cavalieri et al., 1996	Monthly rate of change in sea ice coverage
Chlorophyll a	SeaWifs, MODIS	9km, monthly	NASA, 2016	Aggregation to 0.25°
Wind speed	ERA	0.25°, 6hours	Dee et al., 2011	Monthly average

SOCAT was used for tuning the model and LDEO was used for validation, while the two dataset was largely overlapped. This is not allowed for developing a sound and solid approach.Randomly picking data from SOCAT for calibration, and then removing those data at the same location when picking the LDEO data for validation, would not be too hard to do.

[2] As mentioned by the reviewer, the SOCAT and LDEO databases have a large overlap, and the two datasets cannot be considered independent. In order to remedy to this problem, we followed the reviewer suggestion and created two datasets based on SOCAT and LDEO which do not contain any common measurements. We used the latest releases of both databases (i.e. SOCATv4 and LDEOv2015) and filtered out all non-coastal data points, as it was already done in the previous version of the manuscript. Under our definition of the coastal zone, SOCATv4 contains ~8 10^6 data points and LDEO ~5.6 10^6, over 70% of which are also part of SOCATv4. We then randomly assigned each of those common data points to either database, thus insuring that each data only belongs to one dataset. In the updated manuscript, the new datasets are then called SOCAT* which is used to train the SOM_FFN, and LDEO* which is only used for validation purposes. In the new manuscript, the procedure used to create SOCAT* and LDEO* will be detailed in section 2.2 (Data Sources and processing).

The use of a more robust validation did not alter significantly the performances of the SOM_FFN and, combined with the inclusion of wind speed as a new predictor, the biases and RMSE generated by the model when compared with LDEO* are actually slightly lower than those presented in the original simulations (see table below). Also, note that the use of SOCATv4 and LDEOv2015 provides a significant number of data for the year 2015, which motivated us to expend our simulation period from 17 year to 18.

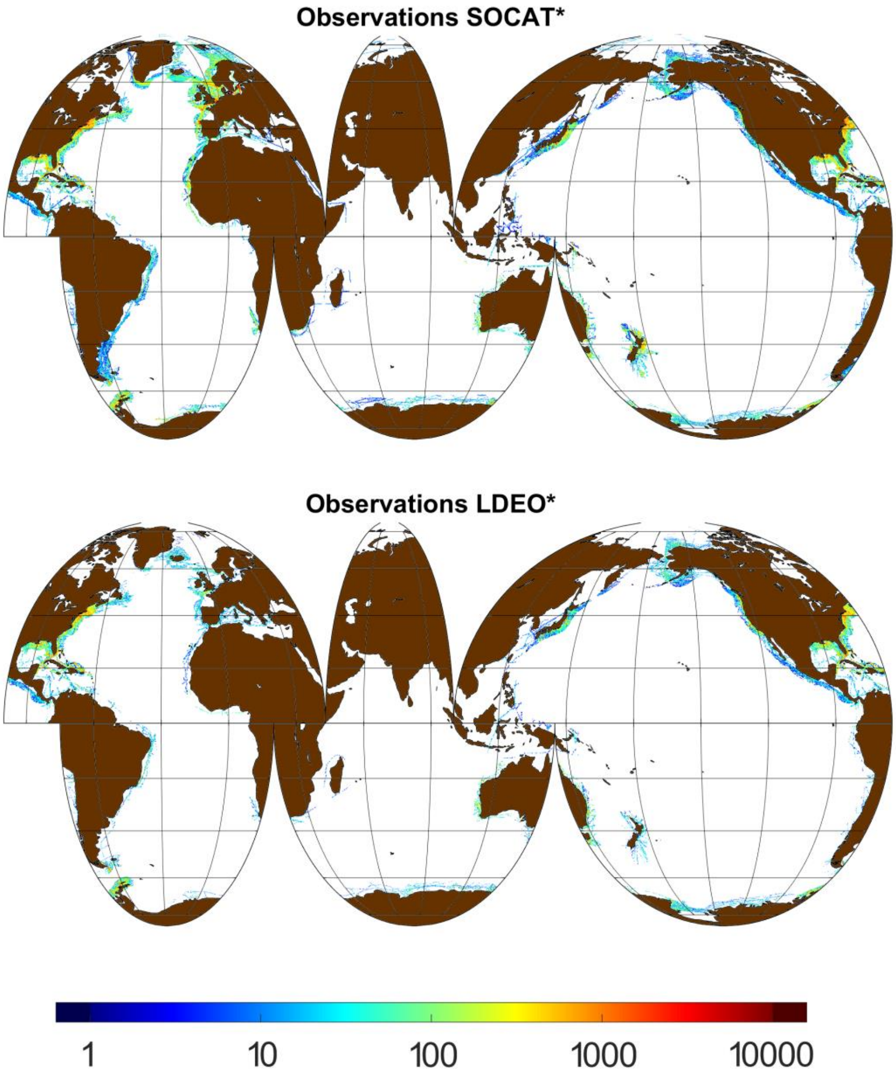

Figure: Number of observations contained in each 0.25° grid cell of the SOCAT* (top) and LDEO* (bottom) databases.

"Table: Root mean squared error between observed and calculated pCO_2 in the different biogeochemical provinces. The SOM-FFN results are compared to data extracted from the SOCAT* and the LDEO* databases.

	SOCAT*		LDEO*	
Province	**Bias (µatm)**	**RMSE (µatm)**	**Bias (µatm)**	**RMSE (µatm)**
P1	0.0	19.1	2.0	20.5
P2	0.2	24.7	1.3	27.2
P3	-0.3	16.1	2.3	22.7
P4	-0.2	31.2	-1.6	33.0
P5	0.0	34.2	-1.4	38.0
P6	0.0	24.3	1.3	27.9
P7	0.1	37.2	-0.2	52.5
P8	0.2	46.8	3.9	51.4
P9	-0.1	23.0	-2.5	33.4
P10	0.0	35.7	1.6	53.1
Global	0.0	32.9	0.0	39.2

The target of this manuscript is not clear. Based on the title, it looks that it is talking about a new product. As to the text, methods and validation are vague, while the authors are still eager to describe the seasonality and spatial distribution, but with no way to go into depth. And maybe because of no full confidence in the results, they frequently warned "considered with caution". I would suggest the authors focusing on method and validation, teasing each detail carefully, which would raise the merit of this study. Because one of the most important changes is to include ice, the authors need to show that by including ice, what was improved? What more was acquired/learned?

[3] The manuscript presents monthly pCO_2 fields for the coastal ocean generated by a statistical method that was never applied in such environment. Obviously, a large part of the manuscript is dedicated to presenting the methods (i.e. the modifications of the open ocean set up in order to better capture the dynamics of continental shelves) and we agree with the reviewer that each critical point of the method should be discussed thoroughly. Following his recommendation, we now discuss results obtained with our model ignoring our new predictors (wind speed and sea ice cover) to better quantify their contribution to the accuracy of our results. Similarly, the added value of performing our simulations at the spatial resolution of 0.25° is also discussed using examples such as the ability of our model to capture the plumes of larges rivers such as the Amazon, which produces an area located North of its river mouth characterized by pCO_2 values significantly lower than those of the surrounding waters (Cooley et al., 2007; Ibanez et al., 2015). We believe that this discussion will clearly allow the reader to understand the added value of our approach. In addition, the validation of our results is now much more developed by including maps of mean residuals obtained when comparing the pCO_2 field generated by the SOM_FFN with data from LDEO* and histograms of the distribution of these residuals with each biogeochemical province (see figures below).
However, we also believe that it is useful to thoroughly describe our results in terms of spatial and seasonal trends and not restrict our analysis to comparison against

validation data. One of the main values of our data product is the resolution of the seasonal variations of pCO_2 in regions of the continental shelf that were largely under sampled until now. We thus believe that, although the main purpose of our manuscript is to describe a new coastal pCO_2 data product, dedicating a significant fraction of our results and discussion to the emerging spatial and temporal patterns in the coastal pCO_2 field is justified and relevant. As for our warning that results in certain regions should be "considered with caution": Despite the increasing number of observations collected and the methodological advancements, there are still regions, such as the Siberian shelves, where only few observations exist and our process understanding is limited. Limited observations mean on the one hand limited information to train our model but on the other hand also only limited means to validate our results. This should not be misinterpreted as us having a lack of confidence, but rather us having limited means of validating our results for some areas of the global coastal ocean. With this statement, we wanted to highlight these limitations and help the reader to critically reflect on our results.

Table: Biases and root mean squared error (RMSE) between observed and calculated pCO_2 using only SST, SSS and bathymetry (STB) or SST, SSS, bathymetry and chlorophyll (STBC) as predictors.

	SOCAT*				**LDEO***			
Province	**Bias (µatm)**		**RMSE (µatm)**		**Bias (µatm)**		**RMSE (µatm)**	
	STB	STBC	STB	STBC	STB	STBC	STB	STBC
P1	0.0	-0.2	20.8	21.0	2.4	2.0	21.7	21.5
P2	-0.1	0.1	26.9	27.8	0.5	0.8	29.0	29.6
P3	0.0	-0.5	22.7	21.3	3.0	2.3	27.1	26.8
P4	0.0	-0.2	33.0	33.0	-1.7	-2.3	33.8	33.8
P5	0.2	0.1	52.7	42.2	-1.7	-0.9	56.9	44.5
P6	0.0	0.1	26.8	26.5	-0.5	0.6	28.9	28.0
P7	0.4	0.3	44.3	44.1	1.2	0.3	59.3	58.8
P8	0.1	0.4	82.6	80.0	9.1	9.0	56.3	58.5
P9	0.1	0.9	34.7	36.5	-2.6	-2.8	39.8	41.8
P10	-0.3	0.7	49.8	49.5	-3.9	-3.0	76.5	75.4
Global	0.1	0.2	43.9	42.4	0.0	0.0	48.0	45.0

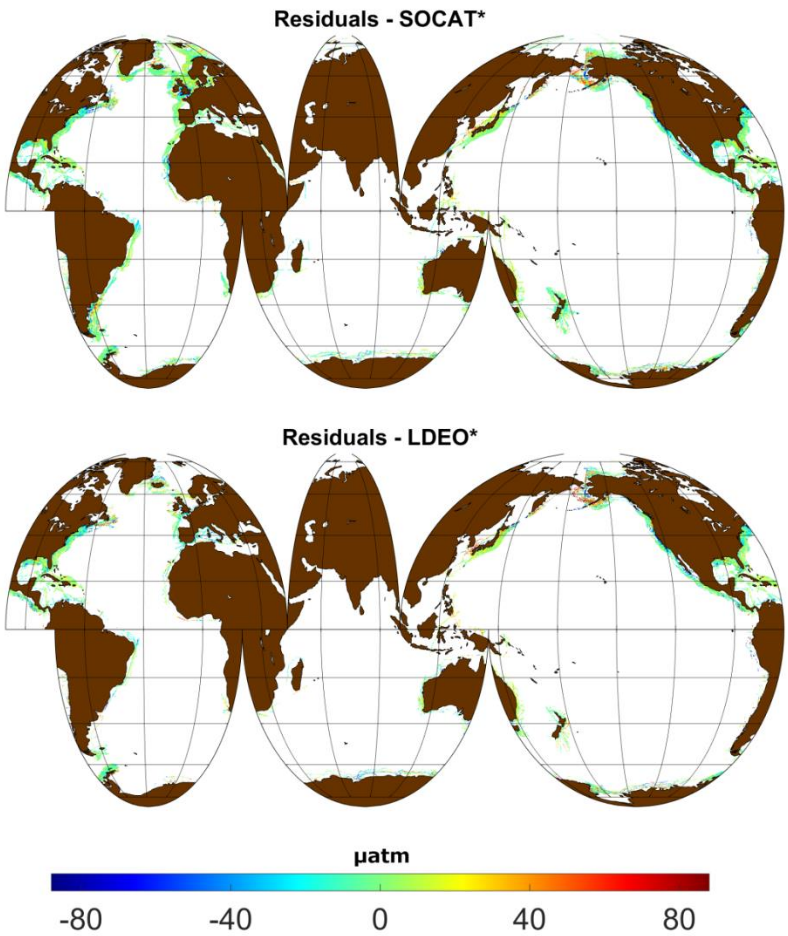

Figure 1: Mean residuals calculated as the difference between the SOM_FFM pCO_2 outputs and pCO_2 observations from SOCAT* (top) and LDEO* (bottom).

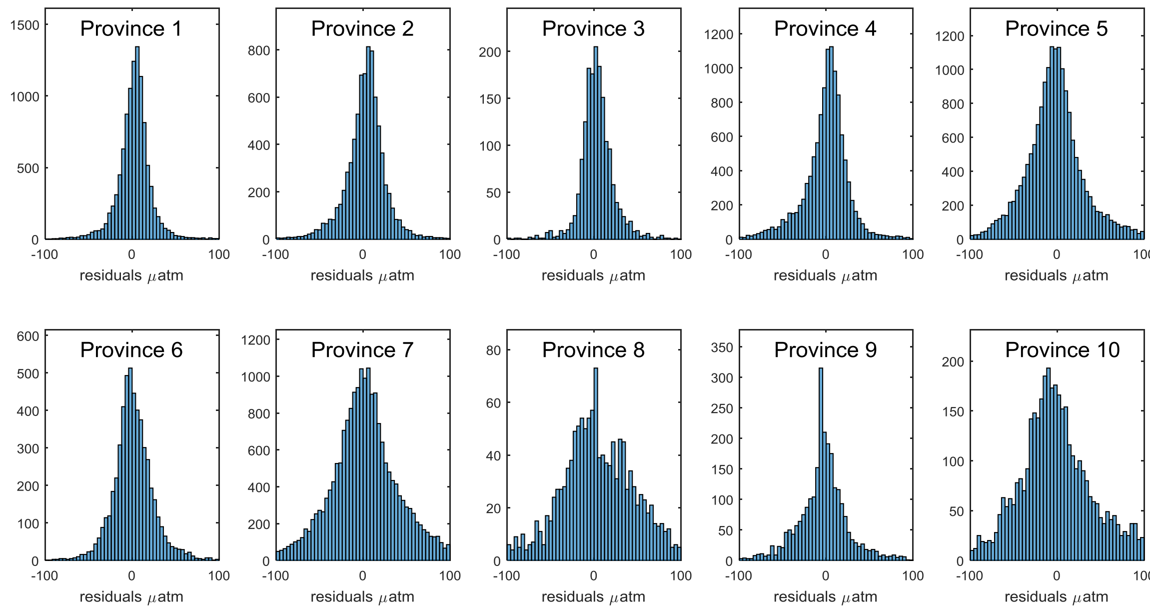

Figure: Histograms reporting the distribution of residuals between observed (LDEO*) and computed (SOM_FFN) pCO_2 in each biogeochemical province.

Specific comments: Abstract- Writing of the abstract needs to be improved. A very clear point should be delivered. People want to know by modifying an established algorithm, what has been acquired/improved and how good it is. Now the authors just say it is assessed using two datasets. Meridional distribution is confirmed. And then talking about seasonality produced from this dataset, which people do not know if it is true or not. If spatial and temporal variability are what the authors concerned, the title should be changed correspondingly.

[4] As mentioned in answer [3], the updated manuscript now dedicates more effort to better identifying what was improved and learned with each of the modification introduced to the SOM_FFN compared to its open ocean set up. Also, we now implemented a more robust validation of our results (following several suggestions of both reviewers), including a revised comparison with monthly climatological cycles extracted from LDEO* at 40 locations (see figure below). We thus do not agree with the reviewer when he suggests that our discussion regarding the seasonality of pCO_2 in coastal waters is unsubstantiated. We not only think that these seasonal signals are supported by our validation but also that the discussion of the seasonal dynamics of the coastal pCO_2 is very relevant to the manuscript and the wider research community. We agree however that the original abstract was not specific enough (especially with respect to seasonal variability) and we will make sure that the updated abstract better reflects the novelty of our approach.

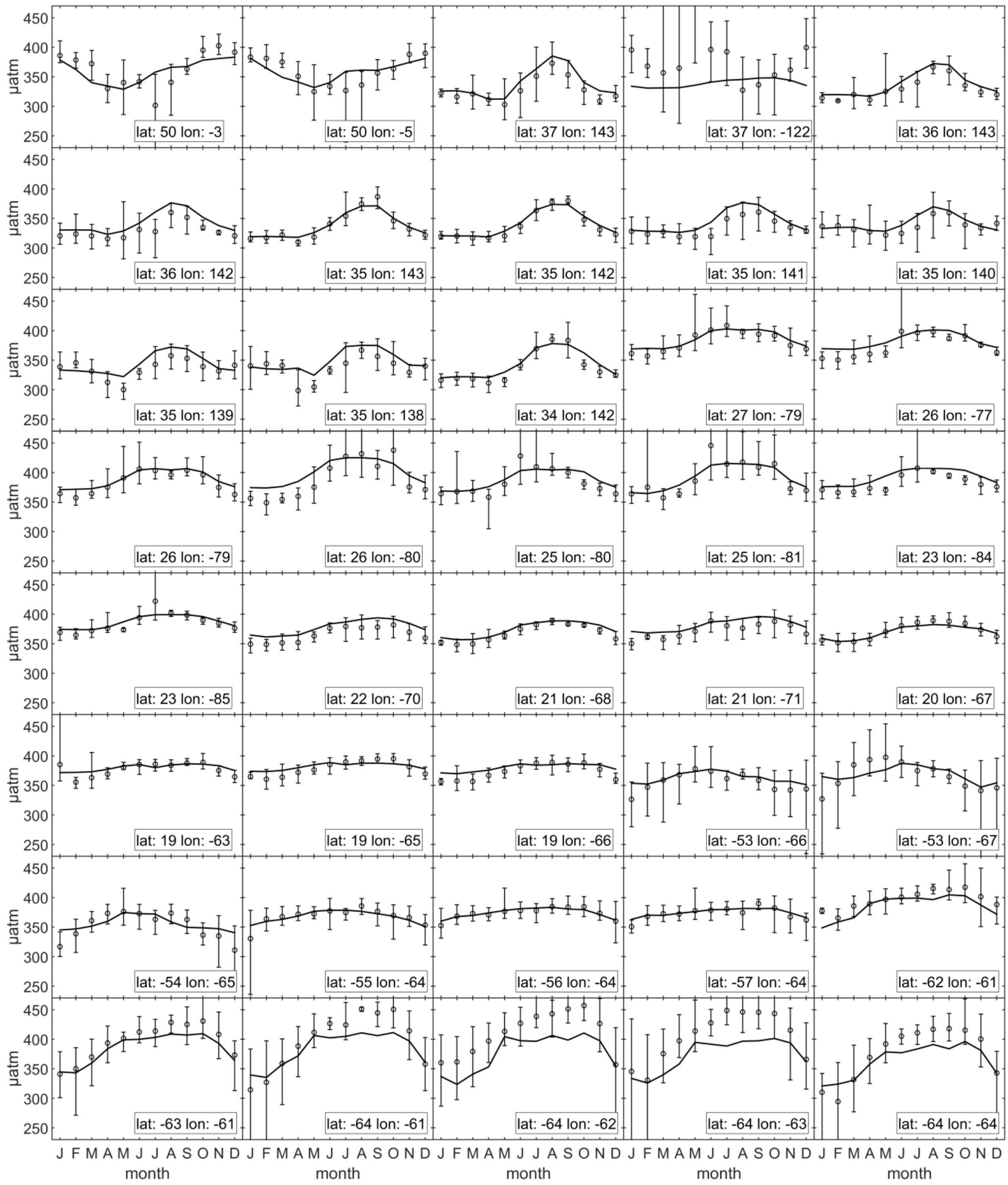

Figure: Climatological monthly mean pCO_2 extracted from the LDEO* database (points) and generated by the artificial neural network (lines) for grid cells having more than 40 months of data. The error bars associated with the data represent the inter-annual variability, reported as the highest and lowest recorded values for a given month at a given location.

Line 36-39, “Overall, the seasonality in shelf pCO2 cannot solely be explained by temperature-induced changes in solubility, but are also the result of seasonal changes in circulation, mixing, and biological productivity.”

This should be well known by everybody. I wonder what it adds to place this sentence in the abstract. It is not clear if it is to explain the seasonality the model produced is not satisfied, or simply to explain the seasonality. One may guess that in the model only temperature was included, so the modeling seasonality can't be explained. But in fact salinity, chlorophyll and sea-ice were all included as predictors in the model, with circulation, mixing, and biological productivity all considered in addition to temperatureinduced changes in solubility.

[5] We agree with the reviewer that all readers familiar with the dynamics of carbon in coastal waters will be aware that the seasonal changes of pCO_2 are not only driven by temperature variations but also hydrodynamics, planktonic productivity etc... The purpose of this sentence was to refer to our analysis of the effect of temperature change on the seasonal cycle of pCO_2 presented at the end of section 3 but we agree that the phrasing was too generic and did not report any new finding. In the updated manuscript, the abstract will be more specific and the outcome of our seasonal analysis more clearly presented (i.e. in which regions of the world, is temperature the dominant driver of the seasonal change in coastal pCO_2, see also answer [4]).

Line 118, it is Landschützer et al. 2015? Should it be 2014?
[6] Indeed, the SOM FFN method is only briefly described in Landschützer et al. (2015) and the reference will be replaced by Landschützer et al. (2014) in the updated manuscript.

Line 141-144, "This approach facilitates future integration with existing global ocean data products (e.g., Landschützer et al., 2016; Rödenbeck et al., 2015) and model outputs, which typically struggle to represent the shallowest parts of the ocean (Bourgeois et al., 2016)". Can you explain what the inner boundary of the global ocean data products is, where they are still confident? I do not think 500 m depth would still be too shallow to struggle. I would think that using 500 m depth as the outer boundary of shelf model would be more than enough (You used 1000 m depth as the outer boundary).
[7] Unfortunately, there is no such thing as a universally accepted inner boundary for ocean data products and models but the extension of their simulation domain varies from one study to the other. The 200m isobaths if commonly used as limit between the open ocean and continental shelves but this limit is somewhat artificial (Walsh et al., 1988, Laruelle et al., 2013). The purpose of extending our outer limit for coastal water as far as 1000m depth is to insure an overlap between coastal and oceanic data product to prevent some regions of the world to remain untreated by either approaches.

Line 152-156, chlorophyll was not included to define biogeochemical provinces using SOM?
[8] Indeed, chlorophyll was not included to define the biogeochemical provinces using SOM, due to the fact that the data coverage is incomplete in the high latitudes in winter due to e.g. cloud coverage. This is the same reason Chl a is excluded from the calculations of provinces P8, P9 and P10 during the Feed Forward Network step. This will be clarified in the text.

Line 185-189, SeaWiFS extends to 2014? Please double-check. To my knowledge, it ends in 2010. By the way, normally people write it as SeaWiFS, not SeaWIFS.

[9] As pointed out by the reviewer, SeaWiFS data do not extend past 2010. The data used later than this date and all the way to December 2015 are taken for MODIS. Also, SeaWiFS will be written as suggested by the reviewer throughout the updated manuscript. This reply will be used to clarify the manuscript and details will be included in the table listing all data sources (see answer [1]).

Line 186, should it be "one of the environmental drivers"?
[10] The sentence will be corrected as suggested.

Section 2.2, it would be better if to appear before the model. Then no need to ask readers to "see below" in Line 164 and 168.
[11] Following the reviewer's suggestion, the sections 2.1 and 2.2 of the manuscript will be inverted, in order to present the datasets used and their processing, before describing the modifications performed to the SOM_FFN.

Line 198, why ice was recalculated? And what kind of recalculation?
[12] The original spatial resolution of the sea ice coverage is days and monthly averages had to be calculated from the original data as well as monthly rates of change in sea ice coverage. This is now explained more clearly in the updated manuscript. In addition, the new table 2 listing all the original spatial and temporal resolutions of all datasets and the manipulations performed with them will help make the data processing more transparent.

Line 211-222 is not evaluation. It is the model training.
[13] Following the reviewer's suggestion, this subsection has been renamed 'model training'.

Line 216, do you mean you used chlorophyll in FFN but not in SOM? Why?
[14] Indeed chlorophyll was used in FFN but not in SOM as justified in answer [8].

I would say that the entire data and method section is really confusing. A cartoon, with input and out clearly indicated, and calibration (training) and validation clearly separated, would help. Also, why twice FFN? The rationale to do this is not clear.

[15] We agree with the reviewer that the different steps and datasets required by our approach may be confusing to the reader and we now improved the clarity of the method in the updated manuscript. In particular, the suggestion of the reviewer to use a conceptual scheme detailing the different steps of the method will be included in the revised ms.
As for the choice of using twice the FFN, it is true that such choice is uncommon and generally not required in a Feedforward Network. Following the remarks of both reviewers regarding this modification, another solution was considered to replace the second neuron layer with the use of a sigmoid activation function bounded between 0 and 1 in the hidden layer. The implementation of this solution did not deteriorate the overall results. The new simulations were thus carried out with this new setting which only uses a single neuron layer.

Line 353-359, this explanation is confusing. There is no reason why results from the global open ocean model can be so different from the coastal model in the overlapped cells. The only critical changes are higher resolution (actually it is an interpolation) and sea ice. Have you tried giving up ice, let other conditions be the same, see what it will be?

[16] As mentioned in answer [1], we do not agree with the notion that our results are just an interpolation of the oceanic model. Other than the spatial resolution and the choice of environmental predictors, both oceanic and coastal models were trained on fundamentally different datasets – the open ocean model was trained with open ocean pCO_2 measurements and the coastal model was trained with coastal pCO_2 measurements. Therefore, we are not surprised that the 2 estimates differ in overlapping areas. However, we do agree that the magnitude of disagreement is somewhat larger than one would expect, highlighting on the one hand current knowledge gaps regarding the coastal to open ocean continuum and on the other hand that more research is needed to close this knowledge gap. The suggestion from the reviewer to perform simulations without the new coastal predictors to quantify their effect is now also included in the updated manuscript, as already discussed in answer [3].

Fig. 2, suggest to use other color, say brown for lands. It is now not easy to tell ice cover from the land.

[17] The suggestion of the reviewer has been implemented in the new version of the manuscript. As an example, all the maps presented in these replies already use a brown colour to represent land.

Literature cited in the responses:

Cavalieri, D. J., Parkinson, C. L., Gloersen, P., and Zwally, H.: Sea Ice Concentrations from Nimbus-7 SMMR and DMSP SSM/I-SSMIS Passive Microwave Data, years 1990–2011, NASA DAAC at the Natl. Snow and Ice Data Cent., Boulder, Colo. (Updated yearly.), 1996.

Cooley, S. R., V. J. Coles, A. Subramaniam, and P. L. Yager (2007), Seasonal variations in the Amazon plume-related atmospheric carbon sink, Global Biogeochem. Cycles, 21, GB3014, doi:10.1029/2006GB002831.

Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U., Balmaseda, M. A., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L., Healy, S. B., Hersbach, H., Hòlm, E. V., Isaksen, L., Kallberg, P., Köhler, M., Matricardi, M., Mcnally, A. P., Monge-Sanz, B. M., Morcrette, J. J., Park, B. K., Peubey, C., de Rosnay, P., Tavolato, C., Thépaut, J. N. and Vitart, F.: The ERA-Interim reanalysis: Configuration and performance of the data assimilation system, Q. J. R. Meteorol. Soc., 137(656), 553–597, doi:10.1002/qj.828, 2011.

Good, S. A., M. J. Martin and N. A. Rayner, 2013. EN4: quality controlled ocean temperature and salinity profiles and monthly objective analyses with uncertainty estimates, Journal of Geophysical Research: Oceans, 118, 6704-6716, doi:10.1002/2013JC009067

Ibánhez, J. S. P., D. Diverrès, M. Araujo, and N. Lefèvre (2015), Seasonal and interannual variability of sea-air CO2 fluxes in the tropical Atlantic affected by the Amazon River plume, Global Biogeochem. Cycles, 29, 1640–1655, doi:10.1002/2015GB005110.

Landschützer, P., Gruber, N., Bakker, D. C. E., Schuster, U., Nakaoka, S., Payne, M. R., Sasse, T., and Zeng, J.: A neural network-based estimate of the seasonal to inter-annual variability of the Atlantic Ocean carbon sink, Biogeosciences, 10, 7793-7815, doi:10.5194/bg-10-7793-2013, 2013.

Landschützer, P., Gruber, N., Bakker, D. C. E., and Schuster, U.: Recent variability of the global ocean carbon sink, Global Biogeochemical Cycles, 28, 927–949, doi:10.1002/2014GB004853, 2014.

Landschützer, P., Gruber, N., Haumann, F. A. Rödenbeck, C. Bakker, D.C.E. , van Heuven, S. Hoppema, M., Metzl, N., Sweeney, C., Takahashi, T., Tilbrook, B. and Wanninkhof, R.: The reinvigoration of the Southern Ocean carbon sink, Science, 349, 1221-1224. doi: 10.1126/science.aab2620, 2015.

Laruelle, G. G., Dürr, H. H., Lauerwald, R., Hartmann, J., Slomp, C. P., Goossens, N., and Regnier, P. A. G.: Global multi-scale segmentation of continental and coastal waters from the watersheds to the continental margins, Hydrol. Earth Syst. Sci., 17, 2029-2051, doi:10.5194/hess-17-2029-2013, 2013.

NASA Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group; (Dataset Release 2016): MODIS-Aqua chlorophyll Data; NASA Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group, 2016.

U.S. Department of Commerce, National Oceanic and Atmospheric Administration, National Geophysical Data Center. 2006. 2-minute Gridded Global Relief Data (ETOPO2v2). http://www.ngdc.noaa.gov/mgg/fliers/06mgg01.html. Accessed 21 May 2017.

Walsh, J. J.: On the nature of continental shelves, Academic Press, San Diego, New York, Berkeley, Boston, London, Sydney, Tokyo, Toronto, 1988.