Summary of Revisions

RC = Reviewer comment

We thank all three reviewers for their positive and constructive feedback. In order to provide a quick overview of the changes to the to-be-revised manuscript, we give a summary here:

- The title has been changed to: "Exploring the ocean and atmosphere coupled system with a data science approach applied to observations from the Antarctic Circumnavigation Expedition" (following RC3.3).
- We have added research questions in the introduction for a framework that better structures the manuscript as a whole (following RC1.6).
- The methods description has been revised substantially to make the language more accessible to non-data scientists (following the general and several targeted comments of Reviewer #1).
- Section 5 (description of individual LVs) will be moved to a new appendix A to substantially shorten the manuscript. We now summarize the outcome of all LVs briefly in a revised section 4.1, and highlight the novel aspects we found there as well. We give give one condensed description of LV9 as example in a revised section 4.2. (following RC1.7, 3.1, 3.4)

RC = Reviewer Comment, AC = Author Comment, new suggested text in blue

Answers to Reviewer 1

Anonymous Referee #1, 28 May 2021

Summary and overall impression

RC 1.1: This manuscript makes use of a large interdisciplinary dataset from the Antarctic Circumnavigation Expedition, a 90-day cruise from December 2016 to March 2017, in combination with the sparse PCA (sPCA) method to extract process understanding from this comprehensive dataset. The study has a very broad scope, aiming to obtain a holistic understanding of the process biogeochemical and physical processes in the Southern Ocean and atmosphere. The method (sPCA), goes beyond standard PCAs, which are commonly used in oceanography and meteorology. sPCAs aim to increase interpretability when dealing with many variables and processes. In addition, the authors apply a bootstrapping approach in order to quantify the uncertainty of their sPCA results.

I find this a very exciting study and it has the potential to be relevant and valuable to the community. I see three main strengths of the manuscript. First, it presents a method (sPCA) that is relatively new in Earth System Science and may be useful for further studies analyzing ship data. Second, the method allows the authors to conduct an extremely multidisciplinary analysis including a broad range of observed variables and are able to extract an understanding of the dominant processes in the study region. Third, the study is based on a new comprehensive observational dataset from a historically under-sampled region (the Southern Ocean), and includes measurements in the ocean, atmosphere, and cryosphere, covering all sectors, different interfrontal zones, both open ocean and near islands and continents, and covering a broad range of physical and biogeochemical variables.

At the same time, I have several major comments that I believe need to be addressed before publication. My main concern is the description of the method. I have to admit that I am not too familiar with standard PCAs, and sPCAs are completely new to me. Assuming that this may be the same for many readers, I believe the manuscript can gain considerable clarity by improving the description of the methods (see general comments for more specific details on this and other major comments).

AC1.1: We thank the reviewer for the positive and very constructive review. Their comments made our study much more targeted, structured, and understandable. We agree that the description of the method was too technical and we have therefore rewritten the text following the major and general comments below. Please refer to our direct answers there.

General comments

RC1.2: sPCA method: I suggest expanding Section 3.1. I would appreciate a discussion on why setting some weights to zero is ok and why this does not lose crucial information. In a standard PCA, we say e.g., 80% of the variability is linked to OV1, 5% each to OV2 and OV3. We then know that there is a remaining 10% of variability due to other processes. With sPCA (the way I understand it from the manuscript) we reduce the complexity, ignoring some variables, to explain all of the remaining variability. Here, we get to 100%, but we actually know that we weighted many variables with 0 in order to do so. Isn't the standard approach more complete in its interpretation? What are the pros and cons of each? It should also be mentioned if the user chooses which weights are set to zero, or if the algorithm does that. (My apologies if I have misunderstood the sPCA method. If that is the case, I suggest you clarify it).

AC1.2: We thank the Reviewer for the valuable comments, these points greatly help in clarifying the methodological sections. We have divided the comment into three points and answer them separately here below.

Point 1 : Is the standard approach not more complete in its interpretation?

The standard approach is only more complete in the sense that in the limit where #LV = #OV, the explained variance will always be 100%, as the Reviewer correctly pointed out. With sPCA, one trades off this full explanation with interpretability, by using an algorithm that sets some OV weights to 0. That is, although standard PCA could explain 100% of the variability, many OV have small associated weights which make it hard to appreciate their contribution to a given LV, whereas forcing the algorithm to set those unimportant variables to a weight of 0, one can safely reduce the amount of OV contributing to a given LV and therefore facilitating interpretation of each LV.

Proposed manuscript change, L163. New text:

"The standard PCA has the ability to extract 100% of the data variance, when considering a number of LVs which is equal to the number of OVs. While at a first glance this might be a strength of the standard PCA, in fact this comes at the cost of having typically a large number of OVs associated with small weights, which makes it difficult to unambiguously select a subset (or cluster) of OVs relevant for a specific LV. By using the sPCA approach presented here, the algorithm instead optimises these weights, so that some are exactly 0. This approach makes it possible to interpret groups of OVs that contribute to any given LV, and their associated strength, by looking at the subset of OVs with a nonzero weight. Note that if one would discard OVs associated with small weights in standard PCA solutions, the explained variance would decrease and there is no guarantee that the resulting LVs are as different from each other as possible, and therefore containing the least redundant information. In practice, sPCA optimises this thresholding process."

Point 2: What are the pros and cons of each?

The main point in favour of sPCA, as opposed to the standard PCA, is the automatic reduction of the number of OVs contributing to the LVs. This has several benefits. The first advantage is the increased ease of interpretation, which is the main motivation for its use in our context. By discarding a large number of OVs, which the algorithm does not deem necessary, to the construction of a given LV, the users only have to focus on a smaller set of input OVs. In our case, by using such a high dimensional and heterogeneous input set, this was a must, because we cannot select which OV features are important in each LV a priori, in an objective and unbiased manner. Secondly, when only few data points are available, the estimation of the data covariance might become an ill-posed problem when many input dimensions are considered. sPCA circumvents this problem by reducing the dimensionality of the estimation problem. This acts as a regularization, which makes it harder for the sPCA to summarize LV corresponding to noise and minor variations, which usually relate to the low variance components of the standard PCA.

These benefits, however, come at the cost of a harder optimisation problem, which does not guarantee that running the method twice will produce the same solution (non-convex), as opposed to standard PCA which generally has a unique solution. To alleviate this issue, and to actually take advantage of this, we developed a bootstrap approach to quantify uncertainty of the sPCA. In addition, since decomposition weights can be 0, LVs could be correlated, although in practice they are close to orthogonal (uncorrelated). This also makes it impossible to summarize 100% of the variance in the same number of components as for the traditional PCA. However, as the algorithm is not forced to do so, noise components and minor variability modes are automatically discarded, making this robustness to noise also a strength.

Proposed manuscript changes:

- L258: Change subsection 3.5 title as "Model limitations and advantages"
- L277, new paragraph: "The main advantage of the sPCA approach over its standard counterpart is the automatic selection of OVs by assigning non-zero weights for a given LV. The automatic optimisation of the weights associated with the OVs is done sequentially for each LV, starting from the one corresponding to the largest mode of variance. This ensures that, although not exactly, all the LVs are as uncorrelated as possible. The use of sPCA has also the advantage of being less susceptible to noise and unimportant data variations. This advantage can be understood when contrasting the sPCA results with the large number of principal components with very low explained variance of the standard PCA. Although by considering these components the standard PCA is able to fully explain the data variance, such variance directions are of little practical use in our case, as it would be difficult to link them to natural processes. Compared to the standard PCA, sPCA is less likely to return components with very small explained variance, which are usually corresponding to noise. This advantage is further strengthened by our novel use of the bootstrap analysis, which promotes robustness to noise, meaning that OVs which contribute mainly through noise are identified as such. Data is resampled randomly, and the influence of noise can be observed in large fluctuations of the solution. Therefore, analyses relying on aggregated bootstrapped solutions are more robust to the influence of noise than the traditional PCA or even a single run sPCA. Moreover, using sPCA over the standard PCA has also the benefit of not being susceptible to rank-deficient covariance matrices, in particular when the number of data points is smaller compared to the number of OVs. And last, but not least, the exploratory character of the sPCA allows researchers to conduct an untargeted analysis and potentially find relationships or (spatial / temporal) patterns which would have been left undiscovered in a targeted analysis because one did not think of the possibility."

Point 3: It should also be mentioned if the user chooses which weights are set to zero, or if the algorithm does that.

In most implementations of sparse algorithms, the user does not manually set the input weights corresponding to the OV, but these are set by the algorithm itself. This is a step that sPCA does automatically, as being part of its internal optimization routine, which aims at maximizing the variance explained by each LV (starting from the first), under the constraint of using a small subset of all available OV. The user usually has indirect control over it, by selecting a hyperparameter controlling the strength of such an effect. We state how we select the hyperparameters in lines 241-247 in the manuscript.

Proposed manuscript changes:

- L163 as for Point 1.
- L161, new text: : " … hence promoting sparsity. Sparsity is obtained automatically as the solution of Eq. 2 leads to the selection of the smallest possible subset of OVs to maximize the variance of the LV."

RC1.3: LVs: I find the current explanation of what an LV is quite confusing (L85-87), which led to further confusion later in the document. I recommend making it really clear here what an LV is in an sPCA and how it is different to the OVs. I recommend explicitly stating that the LVs are the processes we want to understand (i.e., the output from the sPCA) with the help of OVs (i.e., the input to the sPCA). (it becomes clearer later in the document, but is needed early on).

AC1.3: Thanks for the comment. This is indeed an important point, and we clarified it in the text. The Reviewer is correct: LVs are the processes, as estimated by the sPCA algorithm, while OVs are the input variables, i.e. the measurements.

Proposed manuscript changes:

- L87, new text: "… of maximal variance. In practice, LVs can be seen as artificial output variables returned by the sPCA algorithm that are linear combinations of the input OVs, i.e the actual measurements. Therefore, LVs are the target variables that we aim to interpret in this study, where each LV summarises a specific aspect of the data, which we relate to natural processes. This approach has the advantage of reducing the 111 OVs that we measured during the cruise to 14 LVs that we can interpret in terms of the processes that they represent."
- L95, new text: "... sparse weight matrix. The OVs with non-zero weights form a subset (a cluster) of variables that are related to each other and compose a specific LV, which can be interpreted with one or several underlying natural processes.

RC1.4: Please add a section that summarizes what happens during the sPCA to add clarity on the method for people unfamiliar with it. The way I understand how the sPCA works from your manuscript, the user chooses a set number of processes they want to know about (here: 14), feeds all OVs (here: 111) into the algorithm. Some of the OVs are set weighted 0 to reduce the number of OVs for each LV. (→ This should be discussed and mentioned if this happens randomly.) The algorithm then identifies 14 different sets of OVs. The users then see which OVs have non-zero weights in each LV to determine which process each LV represents. i.e. the user has to make a choice: if sea surface temperature, salinity, and MLD are OVs in an LV, then the LV might represent a process linked to ocean circulation. (→ For each LV, it would be good to know which OVs are in it so that the reader can understand how the label for each LV was chosen). We can then also see the percentage of the variability that process has on the variability in all of the 111 variables.

→ Is this correct? If yes, it might give you hints about which pieces of information the reader might want to hear about. If not, my understood explanation might give you hints about which parts were confusing.

AC1.4: The Reviewer is correct in their summary. The only minor feedback we can give, is about the estimation of the weights, which is given in the reply to RC1.1. This is a step that sPCA does automatically, as being part of its internal optimization routine: maximize the variance explained by each LV (starting from the first), under the constraint of using a small subset of all available OVs.

In the original Figures 6, 7, 8, 9, 10, 11, 12, 13, 15, 16, 17, 18, 19, and 20 in the manuscript we show the weights of those OVs that are larger than 2 standard deviations. In the SI we provide lists of all OVs with non-zero weights for each of the 14 LVs. Note that these figures have been moved to the appendix, following a comment by reviewer 3 (RC3.4).

We also think that adding a summary of the main steps of the overall approach is a good idea, and we did so in Section 3.3 (corresponding to subsection 3.4 in the new version of the manuscript).

Proposed manuscript change:

- Switch sections 3.3 "Data preprocessing and model setup" and 3.4 "Missing data and imputation"
- L247, new paragraph. "Our analysis pipeline can be summarized as follows: First, the measurements are preprocessed as described above in order to obtain the input OVs. Then, for each bootstrap, a random subset of data points is sampled, with replacement. This subset is used to compute an sPCA solution with the settings described above. Once all 30 bootstrap solutions are obtained, we perform the alignment of the principal components described in Section 3.2 and compute the distribution of the weights associated with each OV, the distributions of the LV activations, and the average explained variance per principal component. We then interpret these three outputs of the bootstrapped sPCA to understand the underlying natural processes that cause the variability described by each LV."

RC1.5: Unimportant variables for an LV “are forced to be zero”: could we accidentally lose information here? Is this a subjective choice by the authors or done by the algorithm? This should be discussed further.

AC1.5: As the reviewer remarked, the process of setting weights to 0 does not come without caveats. First, this process is automatically done by the algorithm, so there is as little human bias as possible. Usually, OVs that strongly contribute to a given LV (i.e. to a given variance direction) are assigned a non-zero weight, while OVs that do not strongly correlate with the given LV are almost always assigned a weight of 0, because they are noisy and do not carry substantial information. But there is indeed a risk to lose information for variables “in between”, and in particular for OVs that are undersampled. In order to minimize this risk, in our setting, we use bootstrapping: resampling and estimation of model weights provides a measure for how much the solutions vary, which tells us about the stability of the assignments. The more stable the solution is, the smaller the risk of losing information. However, as the algorithm does not have guarantees to converge to the global minimum of the optimization, we cannot exclude that some minor information is lost. By bootstrapping, controlling the optimization through hyperparameter selection, and performing missing data imputation, we believe that the obtained LVs are stable and as rich in information as possible.

We proposed to change the manuscript as written in AC1.2.

RC1.6:Research Question(s): Another concern is linked to the research question(s) the article wants to answer. It is such a broad study that scratches on so many topics that it becomes a bit blurry in the introduction where this is all going. The way it is currently presented, it appears as a data mining approach of plugging in all the data and seeing what happens. Were there some hypotheses before that you wanted to test? I would find it helpful to add a (couple of) specific research question(s) and build on that in the introduction why we want to know about that. E.g., Is it about the processes? Is it about showing that sPCAs are a good tool? (or both). Are there some processes we are unsure about, which the sPCA might shine a light on?

AC1.6: Thank you for pointing this out. Including some more structure in the manuscript by means of our targeted research questions is a very good idea. We have now included the following in the introduction in l. 42:

"To explore interactions between the Southern Ocean system components, we apply an unsupervised learning method, sparse principal component analysis (sPCA). Application of the sPCA has two objectives: i) conducting an untargeted and therefore more objective analysis of data, where the method is less tailored to the science question as compared to more traditional regression analysis, and ii) to target a set of specific research questions (RQ):

RQ1: Is sparse principal component analysis an adequate tool to extract interaction processes inherent to a heterogeneous and short data set, which describes environmental variability?

RQ2: Is it possible to identify geographic locations ("hotspots") that are common to several interaction processes?

RQ3: Which are the key observed environmental variables that strongly contribute to several interaction processes?

Specific answers to RQ1 are given in section 3.5, with respect to model limitations and advantages, and 6.2, with respect to interaction processes. RQ2 is answered in section 6.1 and RQ3 in section 6.3. Note that we focus on the proof of concept of the sparse principal component method by basing the interpretation primarily on the known processes of the Southern Ocean climate system. New scientific insights from this novel approach are described in section 4.1.

To make the structure of the introduction a bit more evident we introduced the following key words:

L. 43: "Southern Ocean Processes:"

L. 72: "The Expedition:"

L. 82: "Unsupervised learning approach:"

In addition, we would like to point out that one of the key strengths of the sPCA is to allow for a more untargeted and therefore more objective analysis of data, where the method is less tailored to the science question as compared to more traditional regression analysis. Therefore, it arises naturally that our study is not following a clear hypothesis that identifies a specific air-sea interaction process. We also now better clarify this aspect of the analysis in the abstract (lines 24/25):

"The sPCA processing code is available as open-access. As we show here, it can be used for an exploration of environmental data that is less prone to cognitive biases, and confirmation biases in particular, compared to traditional regression analysis that might be affected by the underlying research question."

RC1.7: Linked to my previous comment: it is not clear to me which findings are confirmations of processes we already knew, and which findings are new insights. This should be clarified.

AC1.7: This is indeed important and needs more highlighting. We have restructured the manuscript significantly, following this remark and that of reviewer 3, RC3.4. Now all of section 5 has been moved to appendix A. We keep part of the text from former section 5.8 and moved this up to section 4.1. Section 4.1 is now "Short summary of all latent variables and new insights". and contains the text here below, which is merged from the original section 4.1 first paragraph and section 5.8 "Short summary of all latent variables", and contains new additions to highlight the new insights. We also provide a condensed description of LV9 in a new section 4.2 to give one prominent example with new insights. We highlight the new text in blue.

"Figure 3 shows the time series of the 14 LVs, where the blue dots indicate the average of the principal components of the bootstrap runs and the shading indicates the 95% confidence interval (±2 standard deviations). The 14 LVs can be related to physical, biological and/or chemical processes, or changes in the environment that influence the variance of OVs within each LV. We name each LV according to the process or environmental condition, which they reflect (Table 2). Overall, the sPCA solution describes 55% of the variability of the 111 OVs. Here we provide a short summary for all LVs, and in section 4.2 an example description of LV9. Detailed interpretations for each LV are provided in Appendix A.

The largest signal by far originates from the large-scale horizontal temperature and pressure gradients that exist between the low and high latitudes. The effect of these gradients on physical properties of the surface ocean and its activity are mostly captured in the two climatic zone signals (LV1 and LV14). The latitudinal temperature and pressure gradients give rise to the meridional advection of cold and warm air (LV3) with implications on cyclone activity (LV13) and the freshwater cycle with the intermittent character of precipitation events (LV4).

The sPCA led to some new insights into the Southern Ocean water cycle. We were able to systematically identify the different modes of variability in the isotopic signal of marine boundary layer water vapour. δ18Ovap and δ2Hvap show significant contributions to climatological signals (LV1) and the RH environment (LV3), while d_{excvap} mainly reflects the contrasting air-sea moisture fluxes in different RH environments. While an excess of precipitation over evaporation is generally thought to cause a relatively fresh Southern Ocean surface (Dong et al., 2007; Ren et al., 2011), surprisingly, our large-scale assessment of concurrent precipitation and salinity measurements does not yield a direct response of the surface ocean salinity to precipitation events. Instead, we here show that variations in surface ocean salinity are driven by the climatological (long-term) patterns set by surface freshwater fluxes integrated over time-scales longer than synoptic events (LV1) and seasonal melting on sea ice (LV9).

We also find a latitudinal distribution of the nutrient availability and its effect on the productivity, which is highlighted in LV11, LV6 and LV8. This confirms, at the largest scale ever reported, nutrient limitation regimes for the subantarctic front, south of the polar front and associated with the island mass effect as previously reported (Pollard et al. 2002; Blain et al. 2007; Cassar et al 2007; Weber and Deutsch 2010). Moreover, the sPCA successfully decouples the high spatial and temporal variability of iron-limited (LV8) and iron-fertilized blooms (LV6) and their dependence on nutrient availability (LV11), helping to identify the macro- and micro-nutrients responsible for changes to the biogeochemistry and microbial community structure and the source of those nutrients e.g. upwelling, aeolian deposition, sea-ice melt.

The method further highlights the effects of diurnal variability of solar forcing on phytoplankton photosynthetic efficiency and trace gas oxidation (LV10) as well as that of the seasonal variation of the solar forcing on dissolved as well as atmospheric trace gas concentrations and seasonal cycle in microbial productivity (LV7). While the sPCA confirmed known seasonal trends for a number of relatively long-lived key atmospheric trace gases (methane, CO and ozone), it produced unexpected results for some of the reactive trace gases, notably isoprene (LV7). This result points towards a complex interplay between the seasonality of emissions (sources) and seasonality of oxidation pathways (sinks), which, coupled with the potential effect of transport from terrestrial sources, paint a very complex picture for atmospheric isoprene in the Southern Ocean. Further future analysis is required to better understand these processes.

The sPCA solution also clearly highlights aerosol sources (especially for INP and fluorescent aerosol) on or in the proximity of islands and continents (LV5), which was previously not as evident (Moallemi et al., 2021). We observe a clear link between wind speed and sea state and the concentration of large sea spray aerosol (LV12), tying them to the most wind-driven regions of the Southern Ocean. In contrast to that, the smaller accumulation mode particles (LV2) are ubiquitous, because of their long lifetime and various source processes contributing to their abundance.

4.2 Marginal sea ice zone and snowfall (LV9)

LV9 has a very distinct regional signal that is mostly active during Leg 2 of the cruise, with a clear peak between 27 January and 2 February 2017 when the ship was going through sea ice while approaching and leaving the Mertz region ([ref to old] Figure 12a and b), explaining about 3.4(±0.6)% of the variance of all 111 variables (Table 2). The largest contribution to this LV comes from the sea ice concentration (C_i), i.e. fraction of surface area covered by sea ice ([ref to old] Figure 12c), which was unusually low during the austral summer season 2016/2017 (Schlosser et al., 2018).

The sPCA highlights four interesting characteristics of the coupled ocean, ice, and atmosphere system in the melting sea ice region. Firstly, positive LV9 periods are associated with a low surface ocean salinity (S_{sw}) and density (sigma0,sw; ([ref to old] Figure 12c). These relatively fresh and light surface waters suggest a stable surface ocean stratification associated with recently melted sea ice, confirming previous observations (Haumann et al., 2016). While other surface freshwater fluxes such as snow and glacial melt could have been responsible for the low salinity surface ocean, the absence of a low delta18Osw in LV9 suggests no significant contribution of these fluxes. A second interesting observation is the large contribution of the wave period (Tm−1,1) to LV9 (([ref to old] Figure 12c), with a significantly longer wave period in the partially ice covered region when LV9 is positive. Therefore, the sPCA confirms that ice floes in the marginal ice zone dissipate wave energy (Squire, 2020; Ardhuin et al., 2020) with a faster rate for short-wave components of the spectrum (Meylan et al., 2018). Thirdly, net community production (NCP) and phytoplankton biomass (Chlafluo) are both positively correlated with LV9. Therefore, the sea ice melt appears to increase the water column productivity most likely through iron fertilization (Lannuzel et al., 2008, 2016), and/or enhanced water column stratification, relieving light limitation (Vernet et al., 2008; Cassar et al., 2011; Eveleth et al., 2017). A fourth aspect of LV9 is the large contribution of snowfall (SR). While a higher snowfall compared to rainfall is expected near the Antarctic coast in summer, it is unclear if there is a link between snowfall and the presence of sea ice in LV9 - an aspect that requires further investigation. However, the sPCA suggests an atmospheric boundary layer over sea ice that is dominated by Antarctic continental air masses near the surface with moist and warm advection aloft (see back trajectories in supplementary information section S4) producing snowfall at times. Antarctic air masses near the surface in LV9 are indicated by the very low abundances of heavy water molecules (delta2Hvap and delta18Ovap) in the atmospheric water vapour (w), and a low carbon monoxide (CO) concentration.

The presence of sea ice thus helps to maintain Antarctic air masses properties over the ocean by forming a barrier between the ocean and the atmosphere, limiting the influence of surface fluxes on the air mass before it reaches the open ocean (see e.g. Renfrew and Moore, 1999). Therefore, the sea ice influences the vertical atmospheric boundary layer structure, possibly favoring snowfall.

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RC1.8: Eddies: One process that doesn’t seem to be covered in this study, but is a known driver behind variability in the Southern Ocean are mesoscale eddies. This should be discussed.

AC1.8: Thank you for pointing out this limitation of our study, which we had not yet discussed in detail. The main issue why eddies are not captured by our analysis is the resolution for two reasons. 1) Most data are sampled only every couple of hours and 2) even if we have continuous measurement for certain OVs, the 3-hour subsampling/interpolation of the sPCA input data would filter all mesoscale (eddy) activity. For example, given a ship speed of about 10kn (about 19km/h), the 3-hour interval translates to a spatial resolution of about 57 km, which is too coarse to capture eddies. At 50degS, the baroclinic Rossby radius of deformation ranges between 10 and 25km (Chelton et al., 1998). Apparently, this is a substantial limitation of our study that is not able to capture mesoscale and submesoscale variability in the ocean and if future studies wanted to focus on the influence of eddy/mesoscale or submesoscale processes, they would need to use a much higher resolution data set. We have added a respective comment to clarify this limitation (l. 982 in the original manuscript):

“Moreover, our study is limited to the spatio-temporal scales of the ACE cruise (single season), the sampling intervals along the cruise track (varies among variables), and the chosen 3-hourly resolution for the sPCA analysis. This limitation has the important implication that we cannot identify variations and processes on longer scales, such as interannual variations, or shorter scales, such as the meso- or submeso-scale. For example, meso-scale eddies that are an important driver of Southern Ocean variability are not resolved by our analysis, because the 3-hour interval (about 57 km if the ship moved at 10 knots) is larger than the Rossby radius of deformation at these latitudes (Chelton et al., 1998).”

References:

Chelton, D. B., deSzoeke, R. A., Schlax, M. G., El Naggar, K., and Siwertz, N. (1998). Geographical Variability of the First Baroclinic Rossby Radius of Deformation. *Journal of Physical Oceanography*, 28(3), 433-460. https://doi.org/10.1175/1520-0485(1998)028%3C0433:GVOTFB%3E2.0.CO;2

RC1.9: Seasonality: Please add a discussion on the fact that the cruise is only 90 days long (i.e., during one season) and that the ship is moving during that time, making it difficult (or impossible?) to conduct a seasonal analysis. The discussion should include why it is possible (or not possible?) to robustly conclude on any seasonal signals with this data.

AC1.9: We agree that conclusions on seasonality need to be further discussed and that the constant movement of the ship limits a detailed seasonal interpretation of signals. We have added the following to the manuscript in l. 983:

"Even though the ACE cruise covered a relatively long time period from late December to late March, the robustness of the derived seasonal signals from this dataset is limited. This limitation arises from the ship's movement, thereby covering a wide range of environmental conditions. Thus, signals on time scales such as the seasonal signal depicted by LV7 need to be interpreted as integrated signals occurring on sufficiently large scales. For example, the seasonal variation of the intensity of solar radiation in LV7 shows a decrease anywhere across the Southern Ocean towards austral fall. We can also attribute a seasonal signal to phenomena which only occur during a certain period and certain location. For example, the melting of sea ice discussed in LV9 only occurred in a limited region at the time of the cruise, but it would have been a much more widespread signal if the cruise had taken place in austral spring when the sea ice cover was more extensive. Therefore, it is important to note that we cannot discuss the full seasonal evolution of the signal, because we only spent a few days in the sea ice region, but the input of freshwater from the melting sea ice emerges as an important seasonal phenomenon in our analysis."

Specific and minor comments to the text:

RC1.10: L. 131: In this section, I would have liked to also find out a bit more about the measurements, e.g., if the ocean measurement are at the sea surface only (same for atmosphere) and I recommend adding a sentence or two stating the nature of the measurements (sensors, air/water/ice samples… were some data collected by platforms other than the ship, such as satellites/planes…?).

AC1.10:

This is a good point. We have added the following information at the end of section 2.1:

"Generally, all atmospheric measurements were taken from either the container or monkey deck, i.e. 15 m and up to 31.5 m above sea level, respectively. Ocean measurements were either obtained from the underway water line, with an intake at the front of the ship at about 4.5 m below sea level, or from CTD casts. Details on the sampling locations are given in the cruise report (Walton and Thomas, 2018), whereas details on the measurement methodologies are given in the supplementary information section S1."

RC1.11: L. 145: It should also be mentioned here (and possibly in the abstract/introduction) that this is an unsupervised machine learning approach (as stated in the Conclusion).

AC1.11: Thank you for pointing this out. We have rephrased the sentence in L. 146 to: "Sparse PCA, an unsupervised machine learning approach, was used to…". In the abstract in l. 9, we added: "Sparse PCA is an unsupervised machine learning method."