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## Exploring the coupled ocean and atmosphere system with a data science approach applied to observations from the Antarctic Circumnavigation Expedition

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The Southern Ocean is a critical component of Earth's climate system, but its remoteness makes it challenging to develop a holistic understanding of its processes from the small scale to the large scale. The Antarctic Circumnavigation Expedition (ACE, austral summer 2016/2017) surveyed a large number of variables describing the state of the ocean and the atmosphere, the freshwater cycle, atmospheric chemistry, and ocean biogeochemistry and microbiology. This circumpolar cruise included visits to 12 remote islands, the marginal ice zone, and the Antarctic coast.

Here, we use 111 of the observed variables to study the latitudinal gradients, seasonality, shorter-term variations, geographic setting of environmental processes, and interactions between them over the duration of 90 days. To reduce the dimensionality and complexity of the dataset and make the relations between variables interpretable we applied an unsupervised machine learning method, the sparse principal component analysis (sPCA), which describes environmental processes through 14 latent variables.

Our results provide a proof of concept that sPCA with uncertainty analysis is able to identify temporal patterns from diurnal to seasonal cycles, as well as geographical gradients and "hotspots" of interaction between environmental compartments. Our analysis provides novel insights into the Southern Ocean water cycle, atmospheric trace gases, and microbial communities. More specifically, we

- identify the important role of the oceanic circulations, frontal zones, and islands in shaping the nutrient availability that controls biological community composition and productivity;
- find that sea ice controls sea water salinity, dampens the wave field, and is associated with increased phytoplankton growth and net community productivity possibly due to iron fertilisation and reduced light limitation;
- elucidate the clear regional patterns of aerosol characteristics, stressing the role of the sea state, atmospheric chemical processing, and source processes near hotspots for the availability of cloud condensation nuclei and hence cloud formation.

A set of key variables and their combinations, such as the difference between the air and sea surface temperature, atmospheric pressure, sea surface height, geostrophic currents, upper-ocean layer light intensity, surface wind speed and relative humidity played an important role in our analysis, highlighting the necessity for Earth system models to represent them adequately.

In conclusion, our study highlights the use of sPCA to identify key ocean–atmosphere interactions across physical, chemical, and biological processes and their associated spatio-temporal scales. It thereby fills an important gap between simple correlation analyses and complex Earth system models.

The paper and links to data are available here: <https://esd.copernicus.org/articles/12/1295/2021/>

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