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Regeneration of CO_2 Satellite Column Data tailored to an Atmospheric inversion Scheme

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Alex Webb[1,2], Hartmut Boesch[1,2], Frederic Chevallier[3]

[1]National Centre for Earth Observation, University of Leicester, Leicester, UK.

[2]Earth Observation Science, School of Physics and Astronomy, University of Leicester, Leicester, UK.

[3]Laboratoire des Sciences du Climat et de l'Environnement, CEA-CNRS-UVSQ, L'Orme des Merisiers, Bat 701, 91191 Gif-sur-Yvette, France.

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Introduction

- Atmospheric CO_2 variations are typically 10 ppm in 400 ppm with variations in XCO_2 typically even smaller (~1%). As a result, small errors in satellite retrievals or in the modelling of atmospheric transport will significantly affect the CO_2 source-sink estimation

- Bayesian atmospheric inversion modelling schemes often assimilate XCO_2 satellite retrievals which similarly use a Bayesian inverse framework, both relying on a priori assumptions

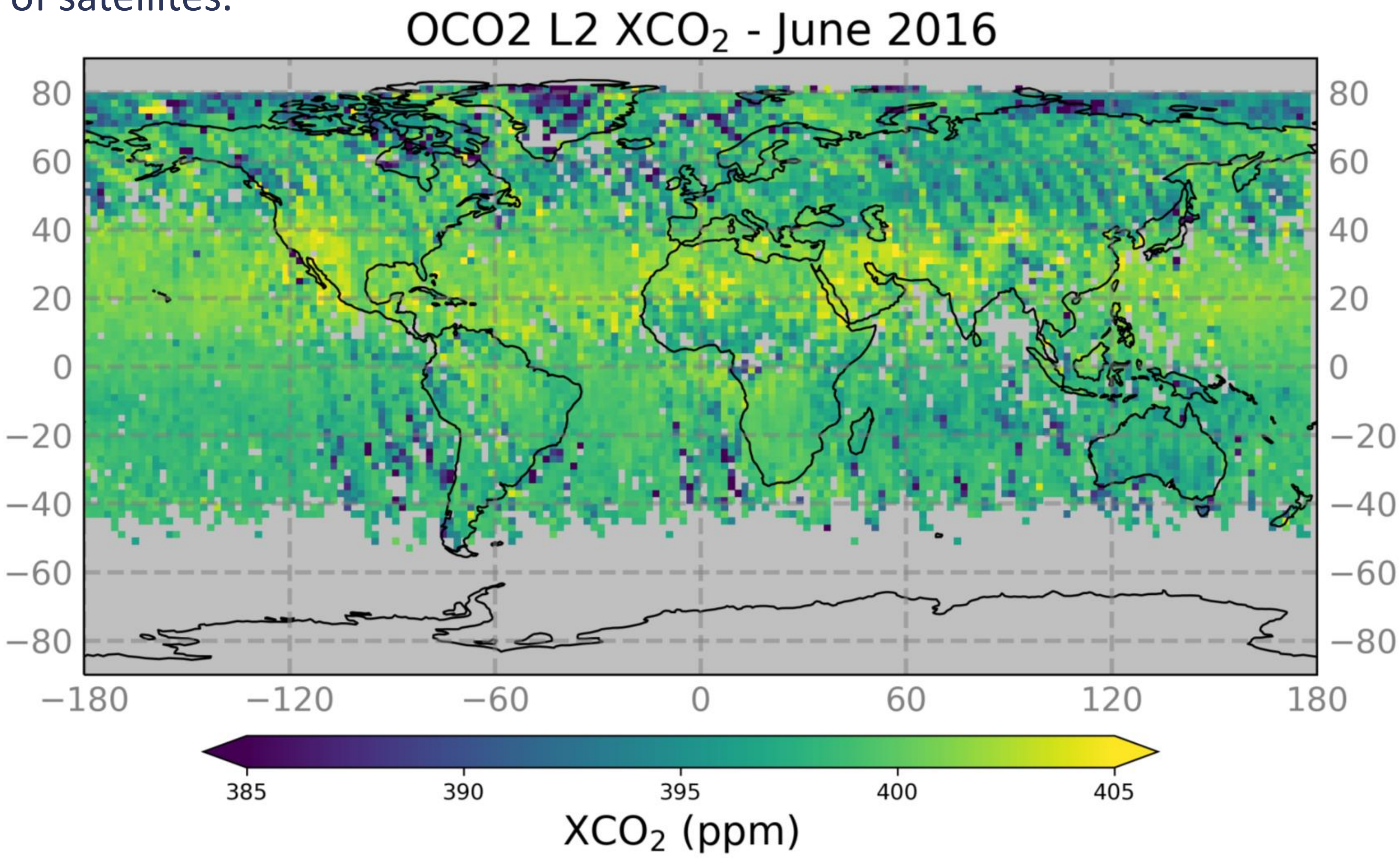
- These assumptions are inconsistent. Models assume a more realistic prior information than satellite retrieval schemes which instead try to maximize the measurement contribution in the retrievals by giving a very weak weight to prior information

- Such inconsistent statistical hypotheses between satellite retrievals and atmospheric inversion schemes may be a significant cause of error in atmospheric inversions assimilating satellite data

- I aim to exchange satellite a priori error covariances with those from an inversion model to derive satellite XCO_2 which is consistent with the specific assumptions of the inversion scheme

OCO-2

- NASA's OCO-2 satellite (Orbiting Carbon Observatory 2) was launched on July 2nd 2014 into a near-polar orbit, joining the A-Train formation of satellites.



- The instrument incorporates three high-resolution spectrometers that make coincident measurements of reflected sunlight in the near-infrared CO_2 near 1.61 and 2.06 µm, and in the O_2 A-Band at 0.76 µm.

- For this study we use OCO-2 L2 Diagnostic 8r XCO_2 data for 2016. The figure shows this for June 2016 plotted to a 2°x2° resolution globally.

Acknowledgements
The OCO-2 data were produced by the OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center.

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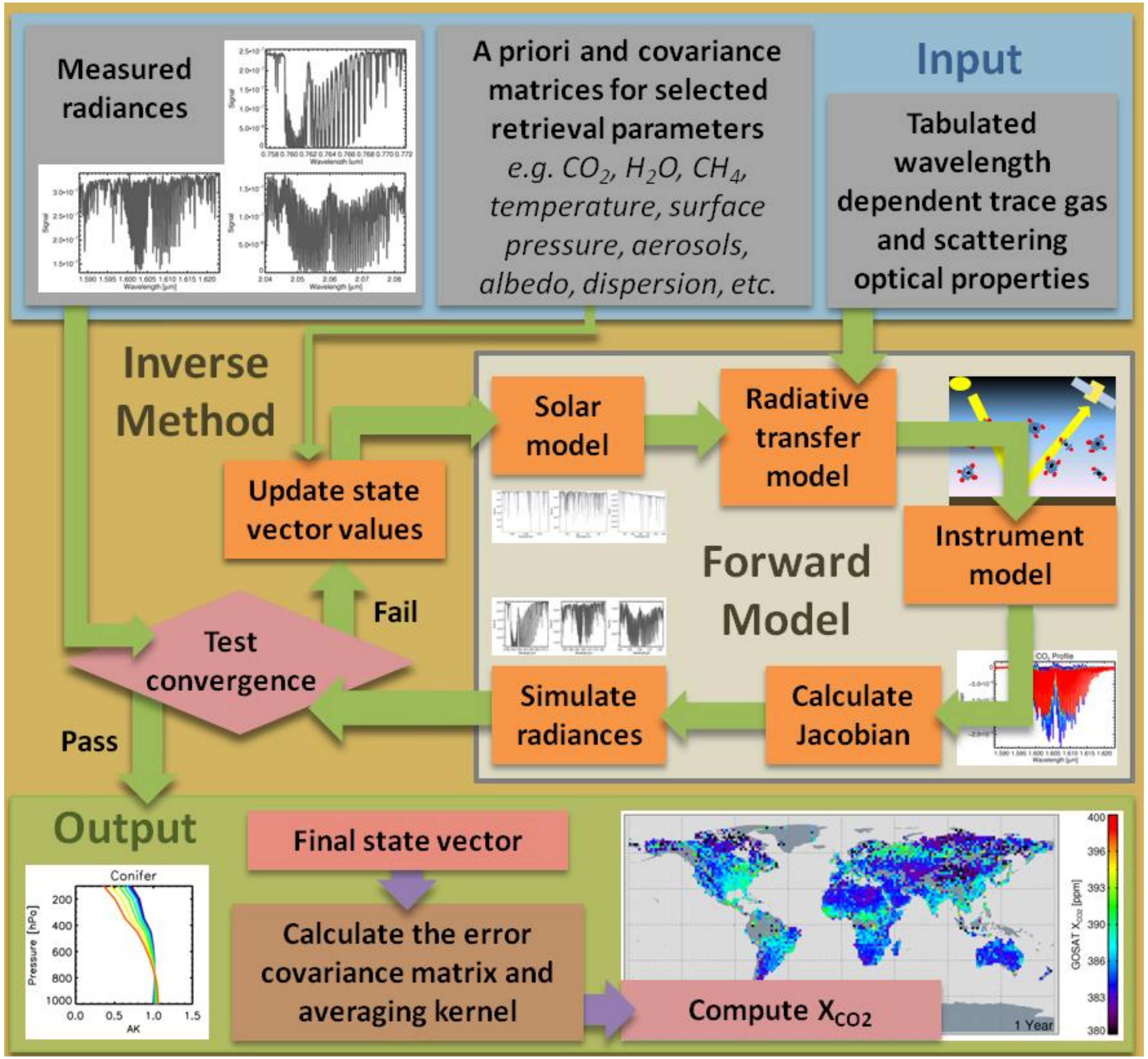
Retrieval Method

- The NASA ACOS retrieval algorithm uses an inverse method with a Forward model.
- A priori data and covariance matrices are supplied to the Forward model which uses a solar model, radiative transfer model and instrument model to simulate the CO_2 spectra.
- We then test these simulated radiances vs the measured (satellite) radiances and use an iterative process to tweak the input parameters in the state vector and recalculate the simulated spectra until it (hopefully) agrees with the measured radiances.
- It is this final state vector which is output, from which the final error covariance matrix and XCO_2 are calculated.

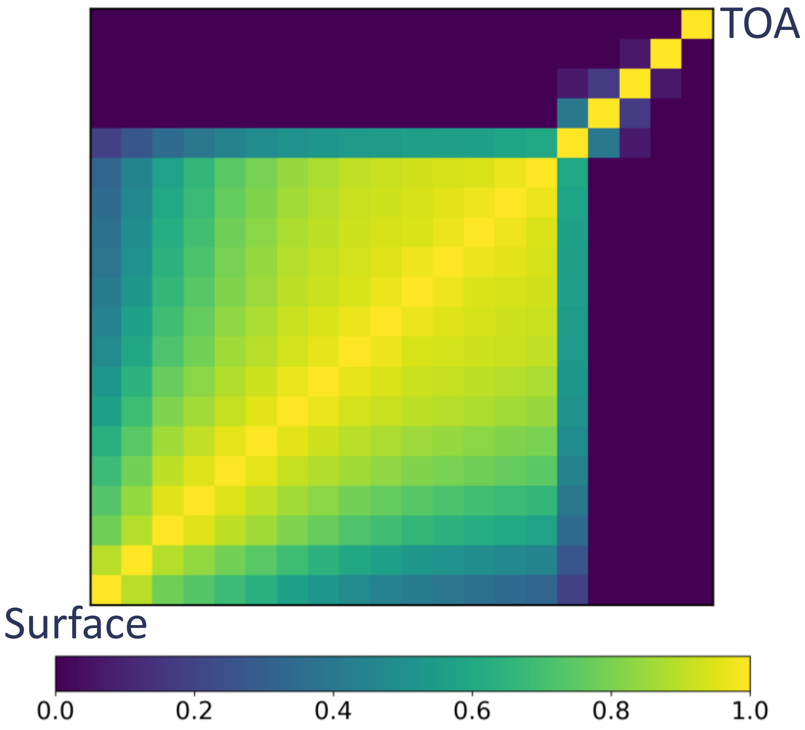


A Priori Error Covariance/Correlation Matrix

- The covariance matrix gives the covariance between two variables off-diagonal and the diagonal elements give their variance. Indicating the direction of the linear relationship between each level in the retrieval profile and every other level.

- I have converted these to correlation matrices which give a measure both of the strength and direction of the linear relationship between two variables.

OCO-2



- The same a priori error covariance matrix is used for all scenes in OCO-2 observations irrespective of land/ocean, month or latitude

- It was calculated by considering the variability of CO_2 weather throughout the profile.

- We see narrow correlations close to the surface which enlarge in the free troposphere. Above 200 hpa the correlations with other levels are close to zero.

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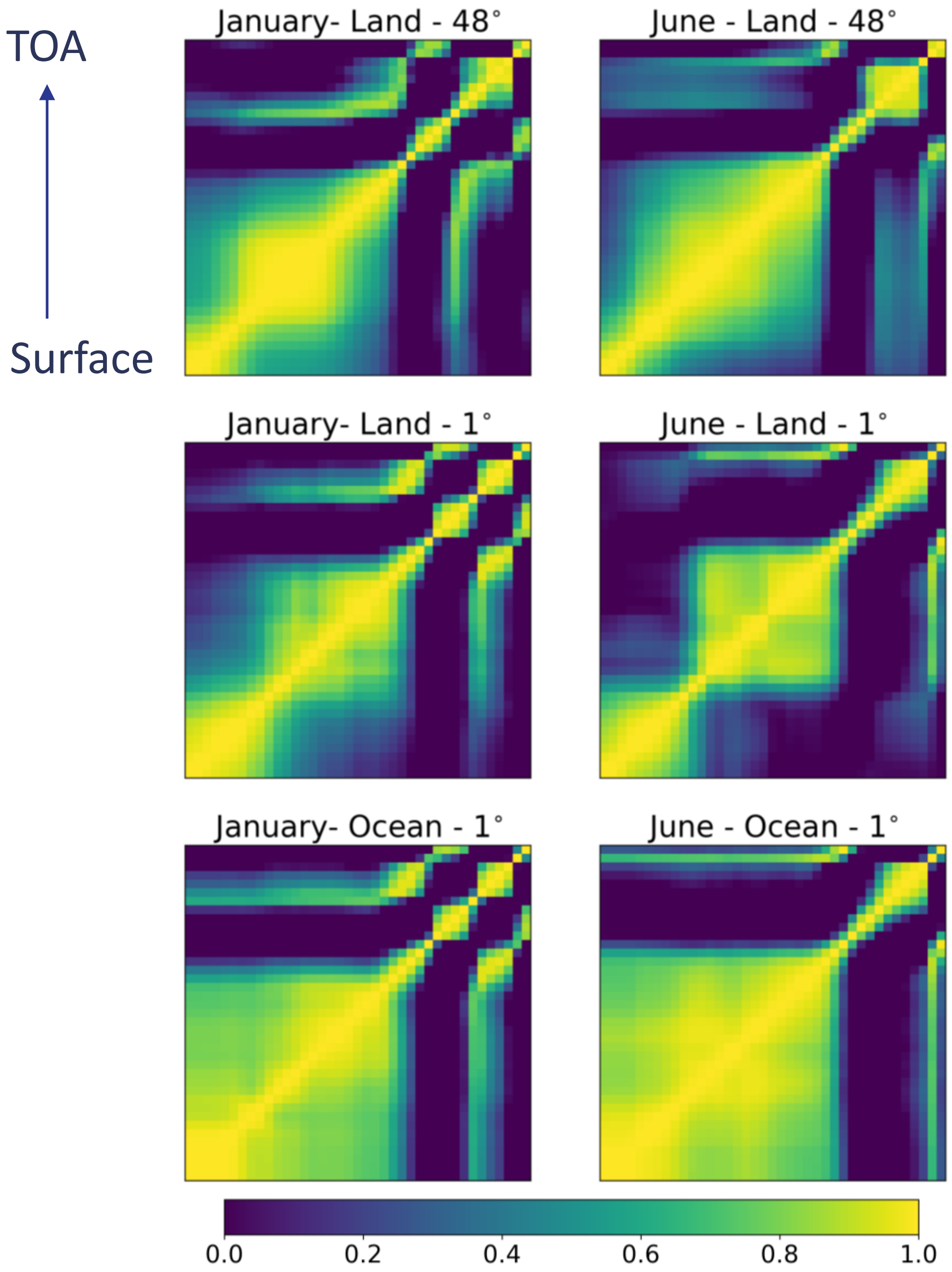
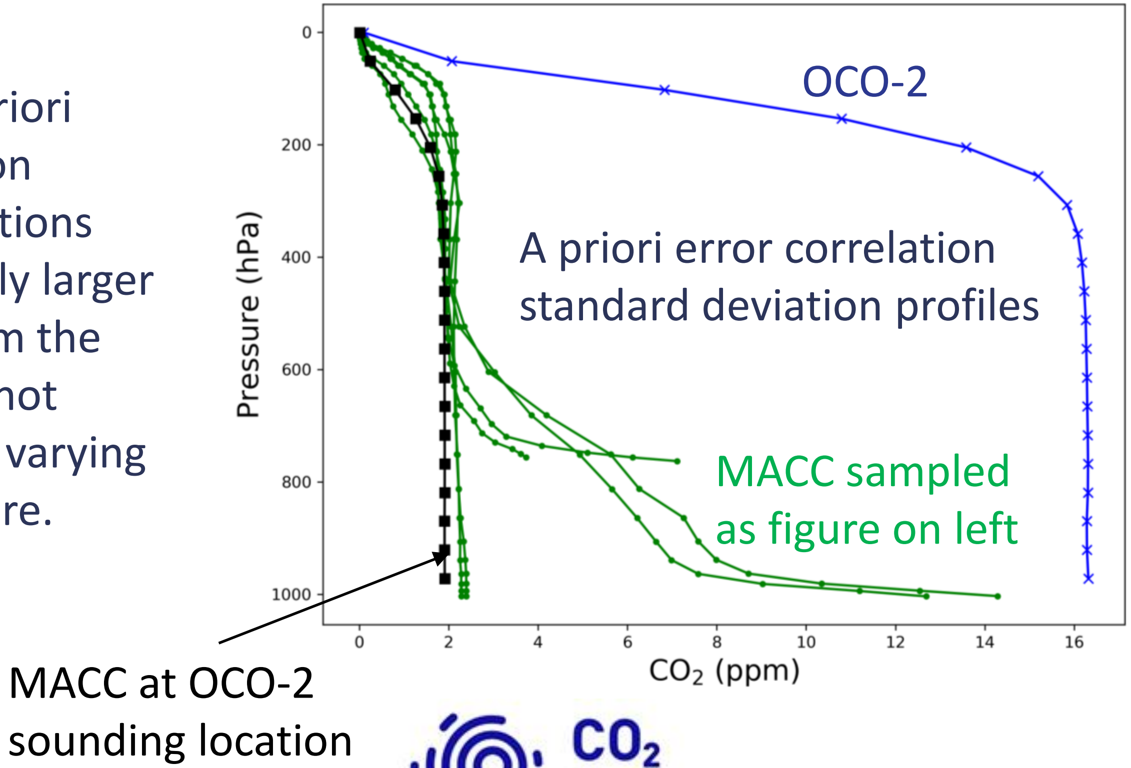
MACC A Priori Error Correlation Matrices



- The a priori error covariance matrices used by MACC are calculated using a fundamentally different method to OCO-2.
- They are constructed to represent the uncertainty caused by flux uncertainties and use a climatology as a function of month, latitude and surface type.
- The OCO-2 a priori error correlation standard deviations are considerably larger than those from the model and do not have the same varying vertical structure.



Methodology

The solution to the inverse problem is expressed in terms of the a priori values, a priori error covariance matrices, Gain matrix, Jacobian, satellite measurements and the error covariance matrices of the satellite measurements

We derive new equations which are entirely in the space of the state vector

These allow us to change the a priori error covariance matrix and obtain a new solution to the inverse problem (framework 1 → 2)

$$\hat{\boldsymbol{x}} = \boldsymbol{x}^{a} + \boldsymbol{G}(\boldsymbol{y} - \boldsymbol{K}\boldsymbol{x}^{a}),$$
$$\boldsymbol{S} = \left(\boldsymbol{K}^{T}\boldsymbol{S}_{e}^{-1}\boldsymbol{K} + \boldsymbol{S}_{a}^{-1}\right)^{-1}.$$

→

$$\hat{\boldsymbol{x}}_{2} = \boldsymbol{S}_{2}\left(\boldsymbol{S}_{1}^{-1}\hat{\boldsymbol{x}}_{1} - \boldsymbol{S}_{a1}^{-1}\boldsymbol{x}_{1}^{a} + \boldsymbol{S}_{a2}^{-1}\boldsymbol{x}_{2}^{a}\right),$$
$$\boldsymbol{S}_{2} = \left(\boldsymbol{S}_{1}^{-1} - \boldsymbol{S}_{a1}^{-1} + \boldsymbol{S}_{a2}^{-1}\right)^{-1}.$$

These new equations have the clear advantage of limiting the size of matrices in solving the retrieval because they don't require the observations, their error covariance matrix, the Jacobian or the Gain matrix.

x - State vector
x^a - A priori value of ***x***
$\boldsymbol{S}_{a}$ - A priori error covariance matrix
y - Satellite measurements
$\boldsymbol{S}_{e}$ - Error covariance matrix of ***y***
F - Forward function linking variables
$\hat{\boldsymbol{x}}$ - Solution to the inverse problem
S - Error covariance matrix of the solution
K - The Jacobian matrix
G - The Gain matrix.

1 – OCO-2 a priori
2 – New framework (MACC a priori)

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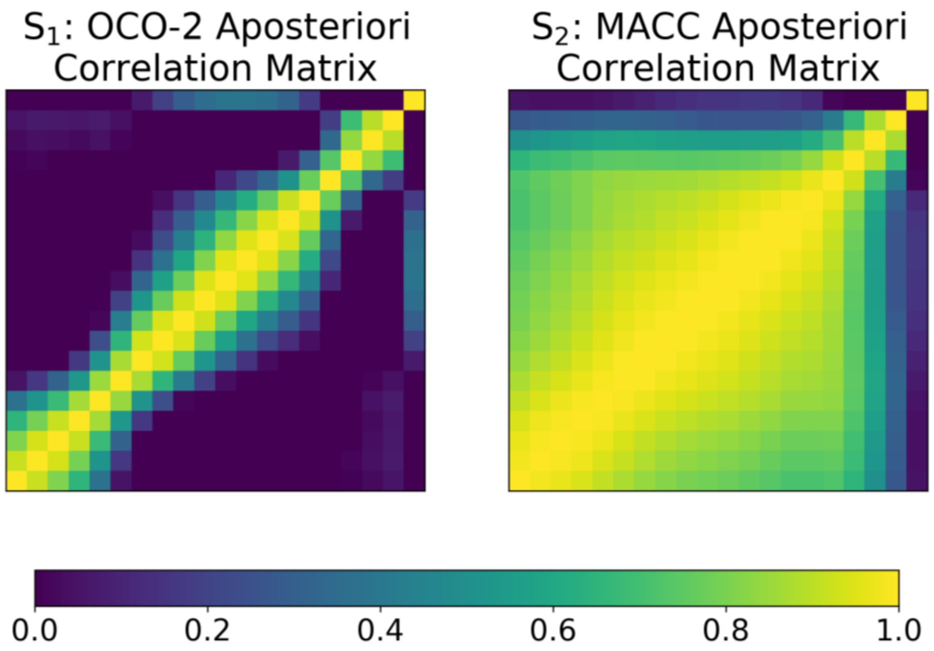
Preliminary Results

- For each of the 70,987,897 clear OCO-2 soundings in 2016, I sample the MACC covariance climatology and resample the 39 level MACC profile onto the 20 level OCO-2 profile

- Apply new equations to recalculate $\hat{\boldsymbol{x}}_2$ and $\boldsymbol{S}_2$ when using MACC a priori covariances instead of OCO-2's

- These CO_2 profiles are converted to XCO_2 values by the method outlined in O'Dell (2012) using a pressure weighting function



- The average difference in XCO_2 between the original OCO-2 data and the recalculated OCO-2 XCO_2 when using MACC a priori error covariance matrices is only $-\mathbf{0.05}$ **ppm** (original – recalculated).

- The average daily standard deviation of global XCO_2 is **4.8 ppm** for the original OCO-2 XCO_2 and **4.3 ppm** for the recalculated XCO_2

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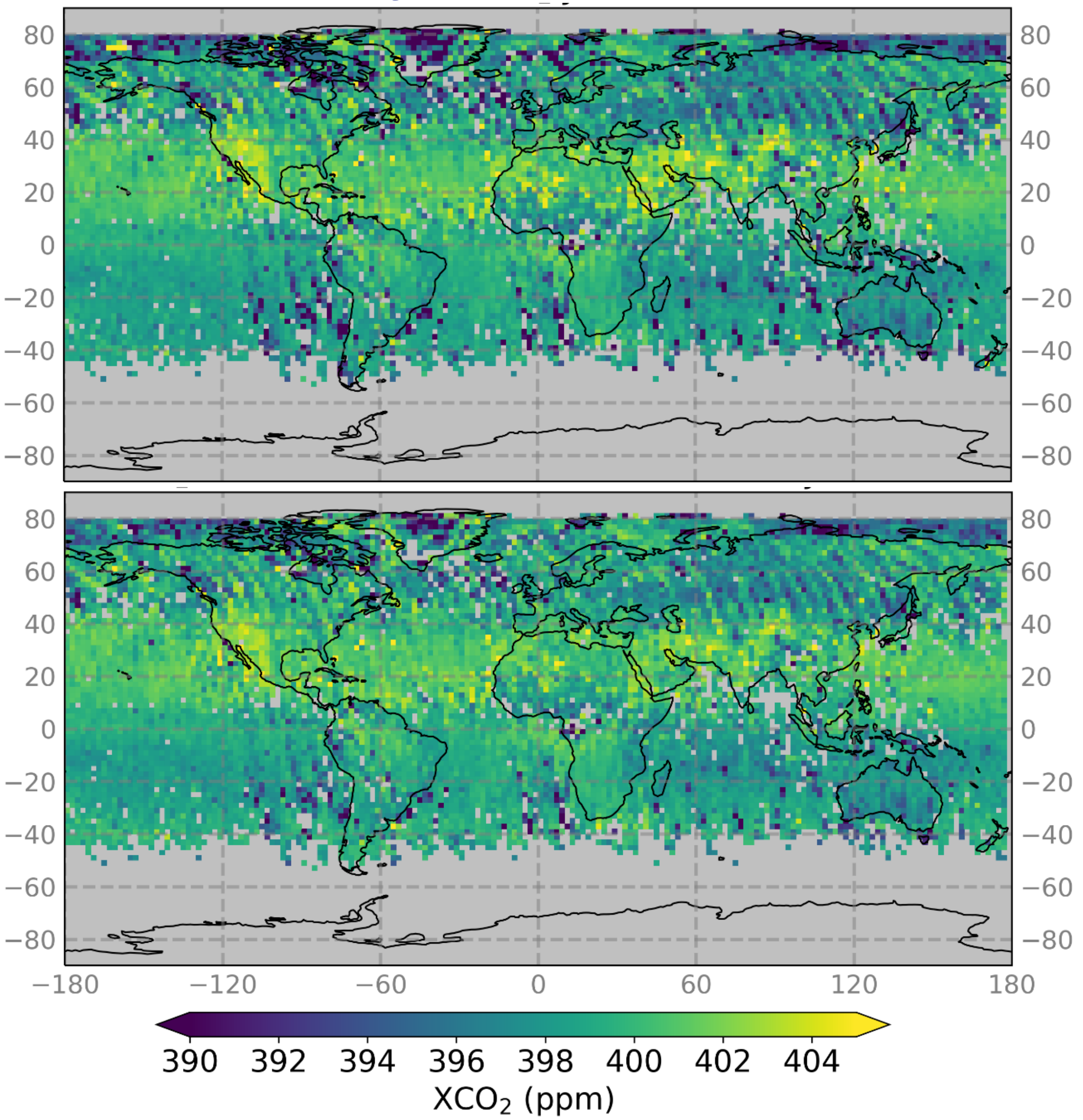
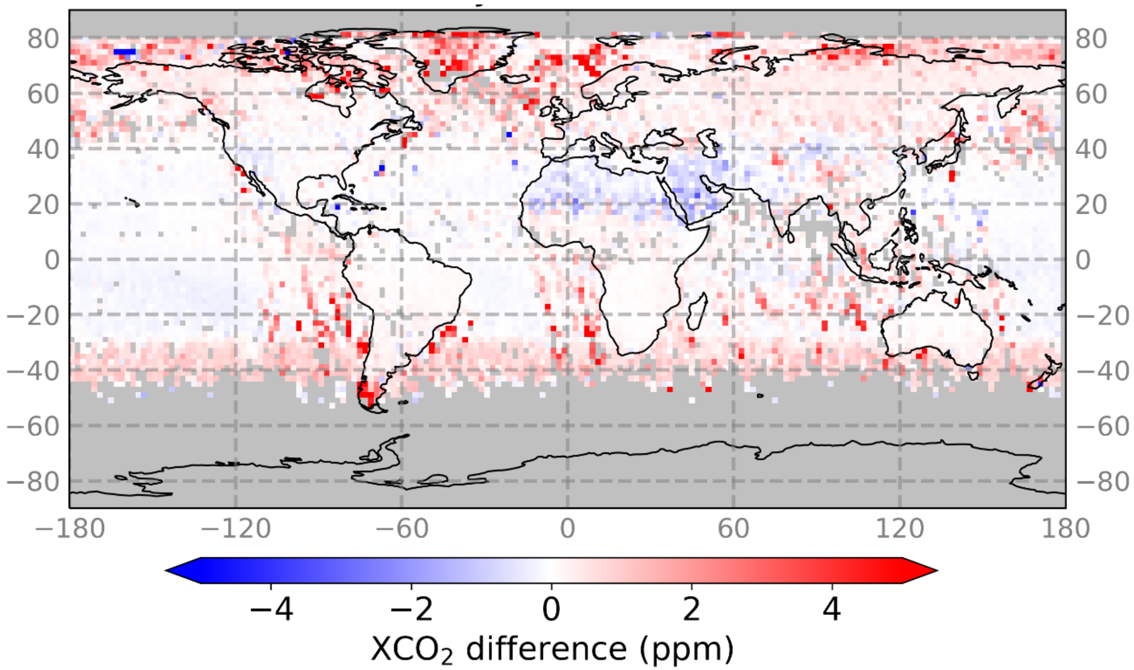


Top left: The original L2 OCO-2 data (June 2016).
Bottom left: The recalculated OCO-2.
Below: The difference (recalculated minus original).



- OCO-2 XCO_2 values are higher in northern Africa and the Middle East, whilst the recalculated XCO_2 values are generally higher away from the equator.

Summary and Next Steps

- We have developed a framework which allows us to make the error assumptions of the satellite retrieval consistent with those of a Bayesian inversion model like MACC.

- This method allows a user to recalculate the state vector with their own prior assumptions, without requiring the observations, the observation error covariance matrix, the Jacobian or the Gain matrix.

- Initial results indicate that the recalculated XCO_2 exhibits regional differences to OCO-2 XCO_2 which merit further investigation.

- Next I need to calculate and apply my own bias correction, since the parameters calculated for the existing OCO-2 data will no longer apply to my data. With this I can compare the results to the MACC model itself and to TCCON ground-station measurements, focusing on the regions where the use of MACC error covariance matrices have the most impact on the results.

- The ultimate goal of the project is to use these modified XCO_2 datasets in the MACC inverse scheme to see if these new results can improve the outcome of the model inversion.