Flux inversion modeling across scales: The Carbon Monitoring System Multiresolution Flux (CMS-MFlux)

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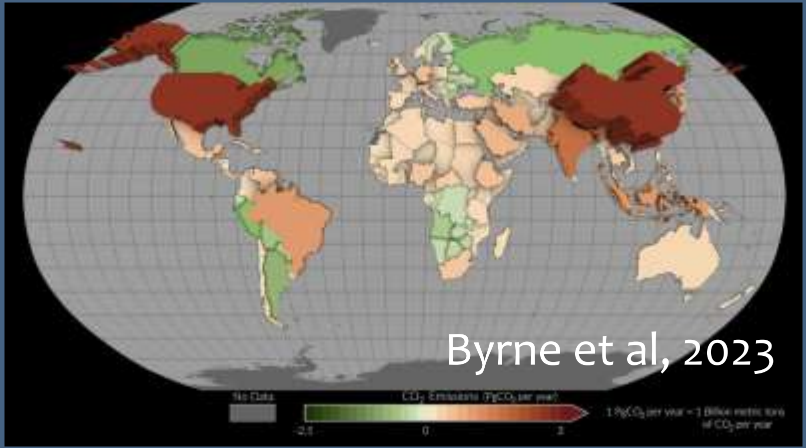
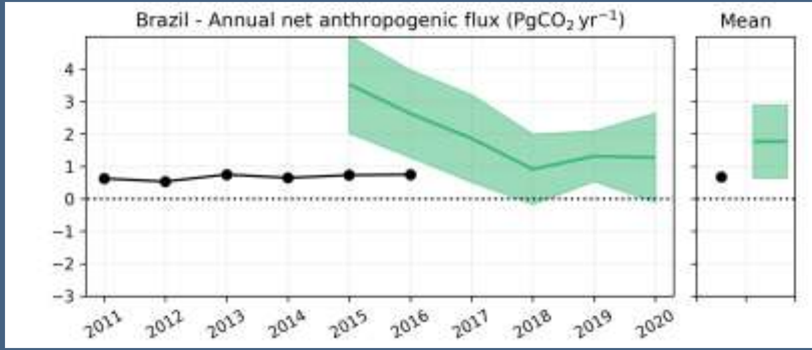
Characterization of inversions: the problem of scale

The OCO-2 MIP and the CEOS Global Stocktake is a bellwether contribution to country-scale net emissions.

- What is the *flux resolution* of an inverse model estimate?
    - When and where do we have information?



Byrne et al, 2023



What is resolution?

How do we quantify the ability to ”resolve” one grid box relative to another?

A robust concept of resolution is well-developed in the remote sensing literature (Rodgers, 2000; Jones et al, 2003; Bowman et al, 2006, etc.)

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \epsilon$$

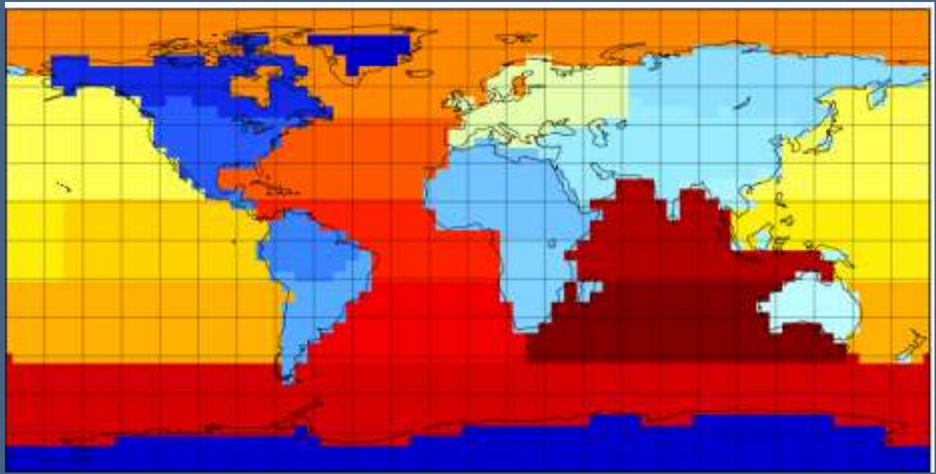
$$\frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} = \mathbf{A}$$

$$\mathrm{dofs} = \mathrm{Tr}(\mathbf{A})$$

4D-var and EnKF systems implicitly have an averaging kernel.
The problem is how to compute it.

The old standard TRANSCOM

- Inverse models minimize the Bayesian cost function.
- Analytic systems are explicit, but with a reduced control vector, **z**.
  - Complete characterization, e.g., averaging kernels and diagnostics
- 4D-var systems are implicit, but with a full control vector, **x**.
  - Approximate error characterization.



Guerney, 2002

$$J(\mathbf{x}) \equiv \frac{1}{2}(\underbrace{H}_{\text{forward model}}\mathbf{x} - \mathbf{y})^T \underbrace{\mathbf{R}}_{\text{model-data error covariance}}{}^{-1}(H\mathbf{x} - \underbrace{\mathbf{y}}_{\text{data}}) + \frac{1}{2}(\mathbf{x} - \underbrace{\mathbf{x}^b}_{\text{prior}})^T \underbrace{\mathbf{B}}_{\text{prior error covariance}}{}^{-1}(\mathbf{x} - \mathbf{x}^b)$$

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{B}^{1/2}(\mathbf{I} + \mathbf{B}^{1/2}\mathbf{H}^\top\mathbf{R}^{-1}\mathbf{H}\mathbf{B}^{1/2})^{-1}\mathbf{B}^{-1/2}\mathbf{H}^\top\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}(\mathbf{x}))$$

Bridging the scales: a multiresolution approach

Start with a coarse basis set (e.g., TRANSCOM) and then build a set of *orthogonal* anomalies

$$f(x,y) = \sum_i \alpha_i \Phi_i(x,y) + \sum_j \gamma_j \Psi(x,y)$$

TRANSCOM

<<Ondelletes>>

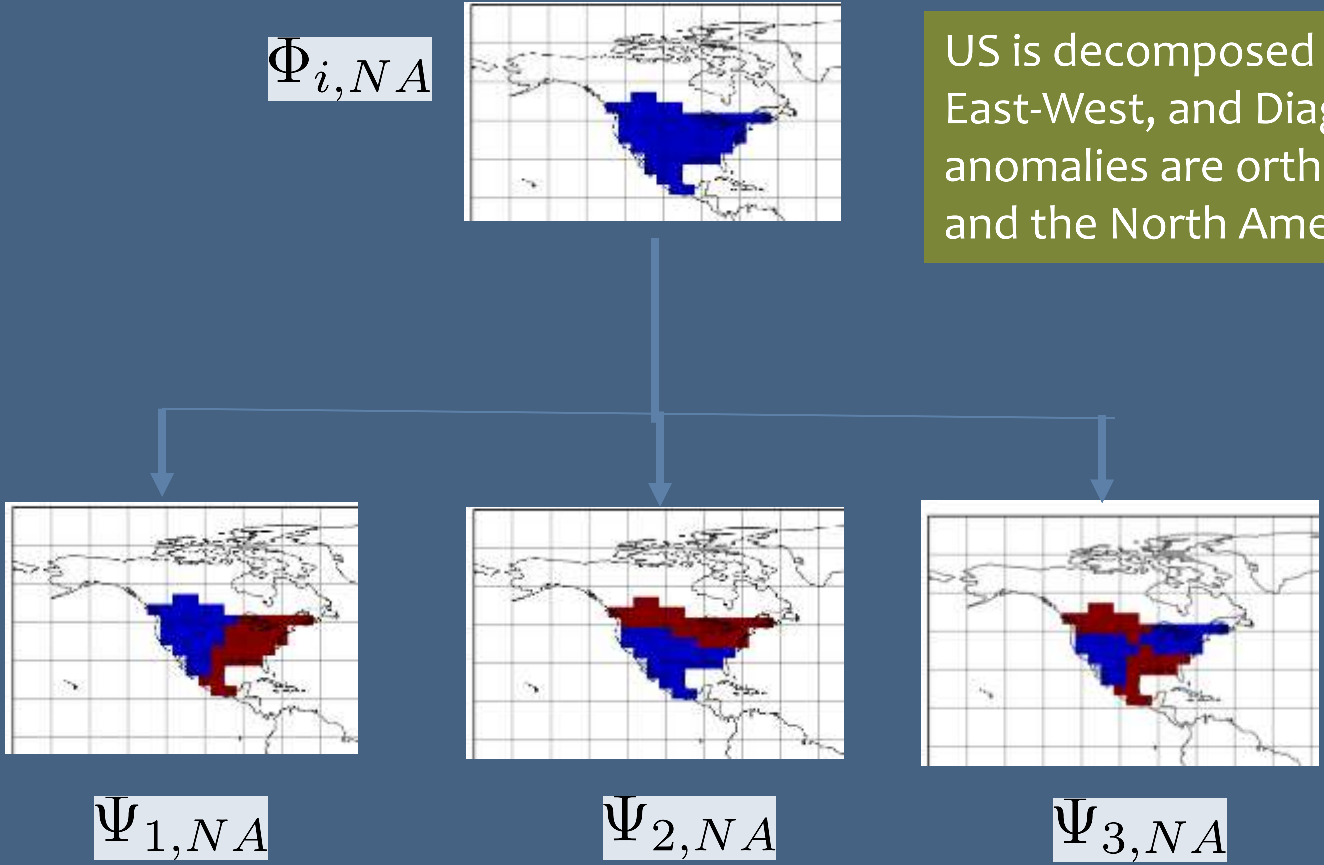
We can write this in vector-matrix format as

$$\mathbf{x} = \mathbf{W}\mathbf{z}$$

This decomposition is *orthogonal*

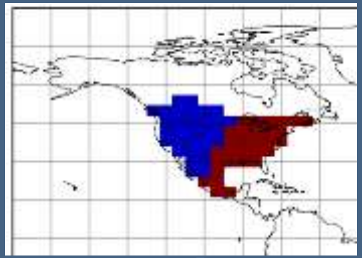
$$\mathbf{W}^\top \mathbf{W} = \mathbf{I}$$

First Multiresolution Refinement



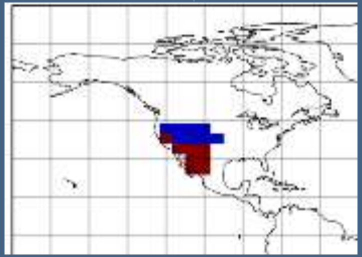
US is decomposed into a North-South, East-West, and Diagonal anomaly. These anomalies are orthogonal to each other and the North American mean flux

Second multiresolution refinement

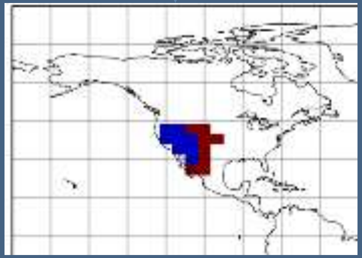


$\Psi_{1,NA}$

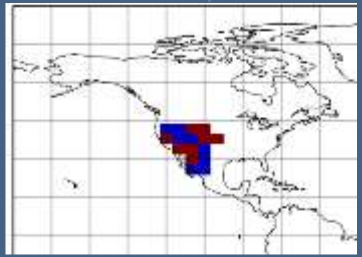
Successive refinements lead to a complete basis set for all grids. Each refinement is orthogonal to each other and upper/lower levels.



$\Psi_{1,1,NA}$



$\Psi_{1,2,NA}$



$\Psi_{1,3,NA}$

Emulation of CMS-Flux with CMS-MFlux

- An analytic solution requires a limited basis set--M<<N wavelets.
- Here, we choose the wavelets that best represent the “support” of CMS-Flux

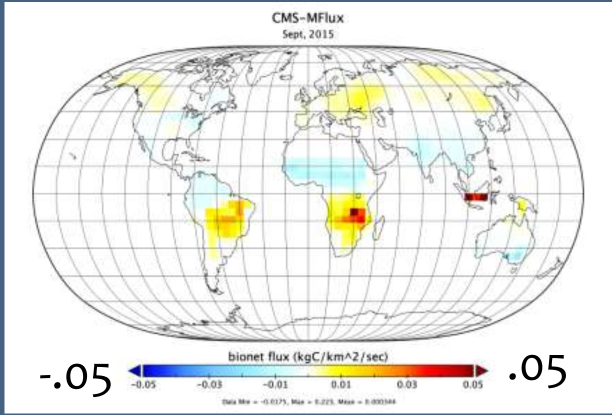
Choose ϕ_i for $$\mathbf{x}_M = \sum_{i=1}^{M} < \mathbf{x}_{CMS}, \phi_i > \phi_i$$

For this case, M ~4000, where N ~ 40000 for one year.
So, about 10% of all available grid boxes.

Adding the scales

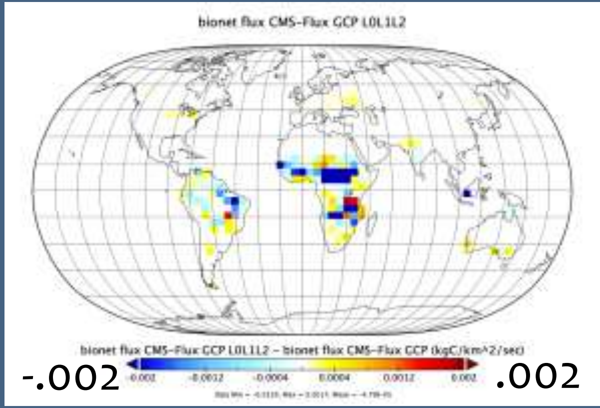
Adding more wavelets enables finer spatial resolution estimates.
Example of fluxes for Sept 2015

CMS-MFlux (all)



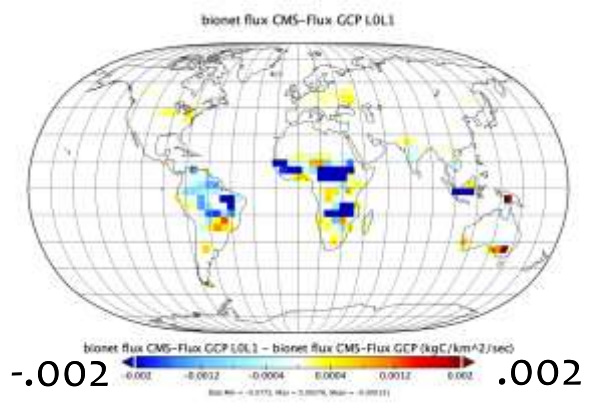
CMS-MFlux (all the scales)
(~325 wavelets)

all- L0→L2



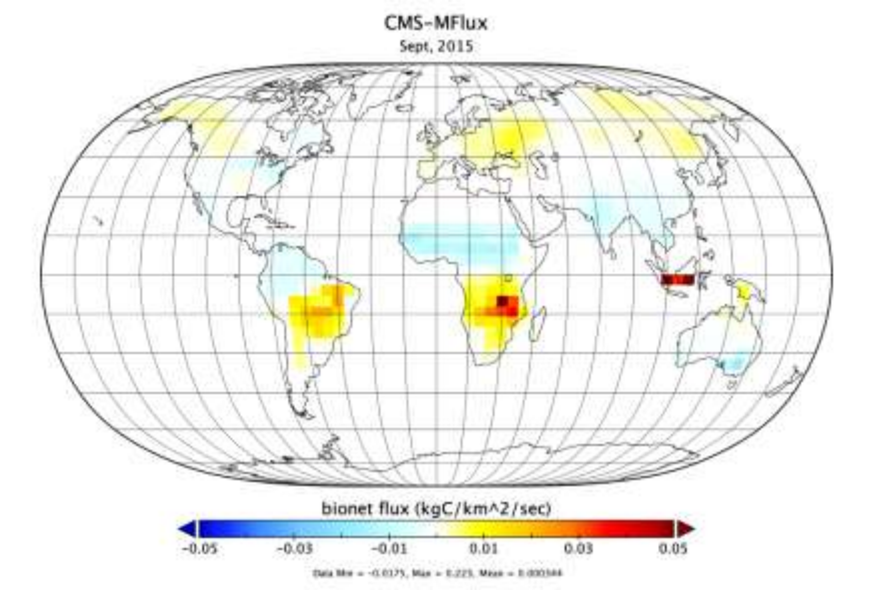
CMS-MFlux - L0+L1+L2
(~135 wavelets)

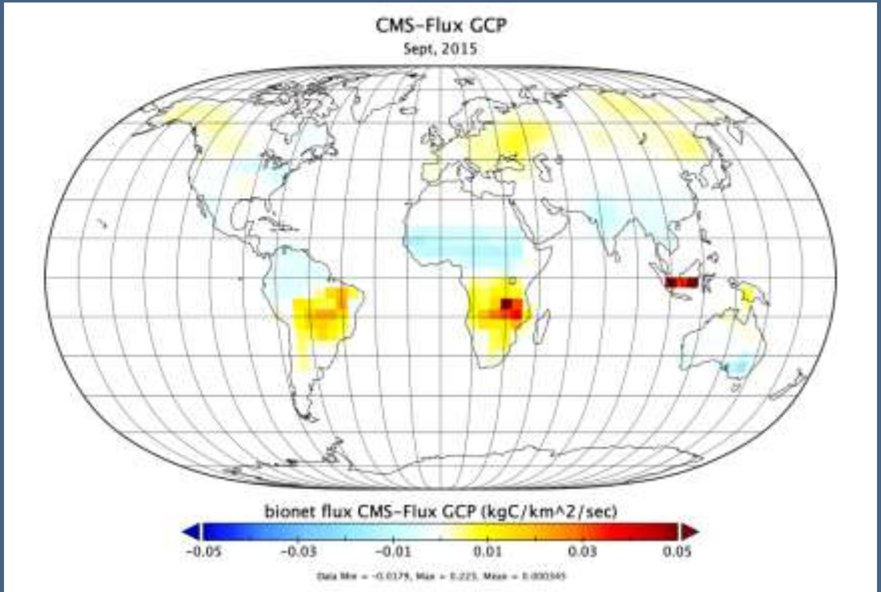
all- L0→L1



CMS-MFlux - L0+L1
(~53 wavelets)

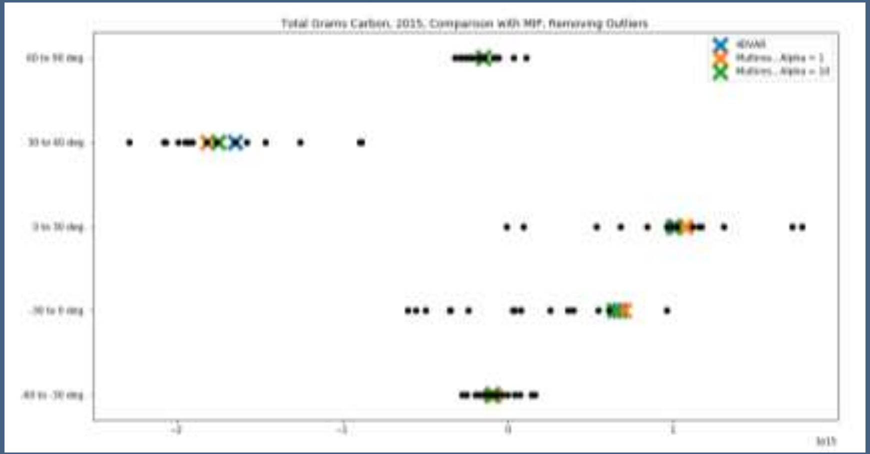
Comparison between CMS-Flux 4D-var and CMS-MFlux

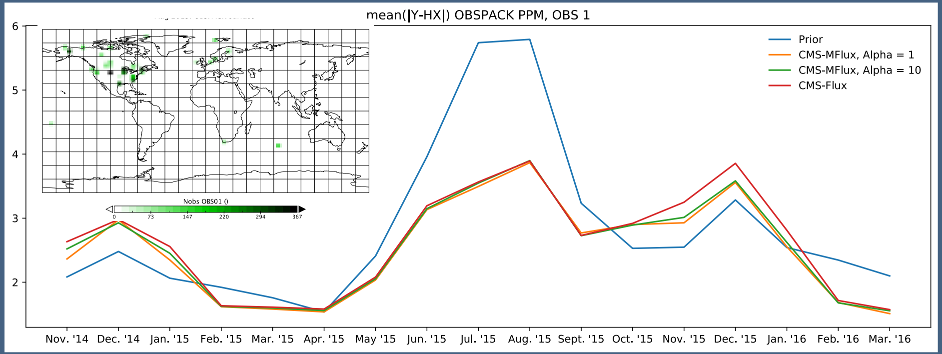




- CMS-Flux and CMS-Mflux use the same assimilation window and priors.
- CMS-MFlux basis and covariance are constructed to mimic the 4D-var solution.
    - Virtually the same flux pattern.

Comparison of CMS-MFlux to OBSPACK and OCO2-MIP

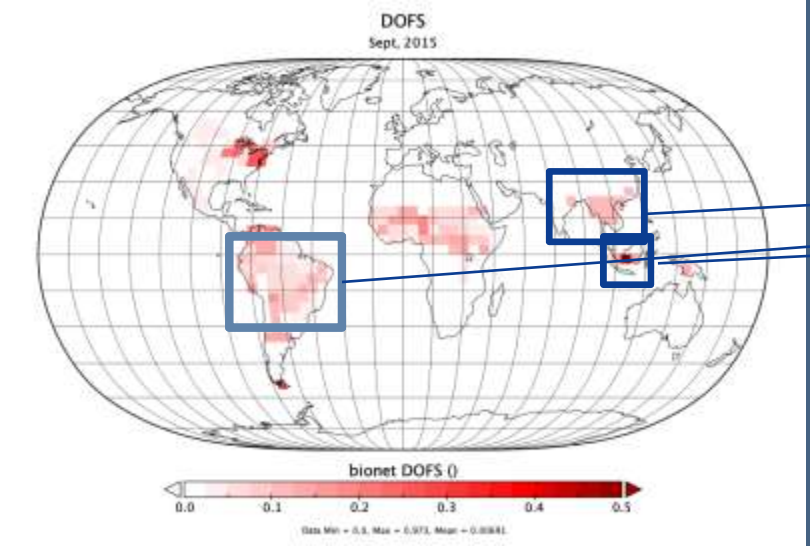


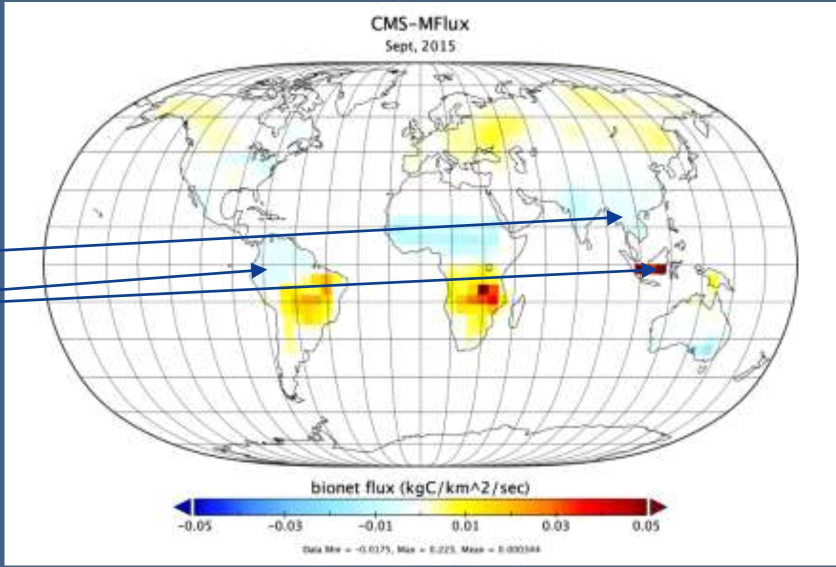


- CMS-MFlux is well within the range of the OCO2-MIP ensemble
- CMS-MFlux and CMS-Flux are in close agreement

- CMS-MFlux is in substantially better agreement to independent observations (OBSPACK) relative to the prior
- Overall good agreement in errors between CMS-Flux and CMS-MFlux

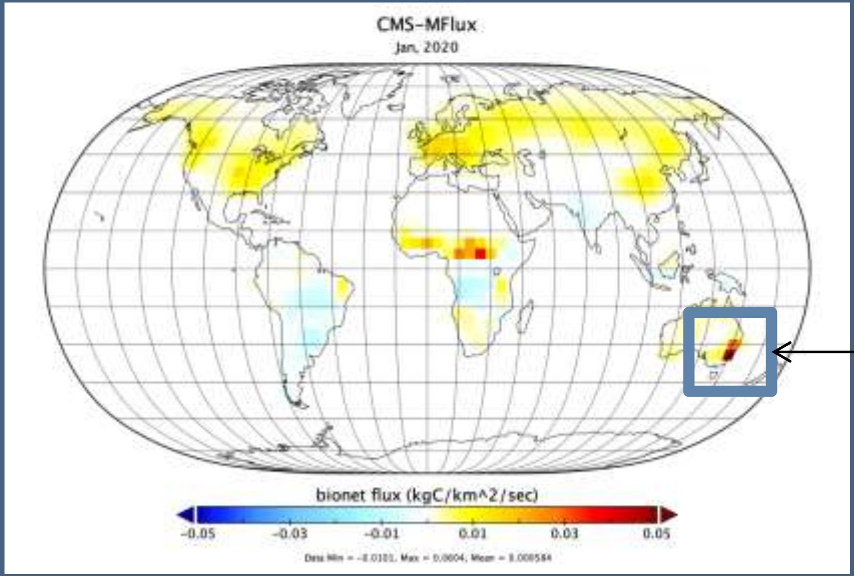
Interpreting the inversion: Averaging Kernel

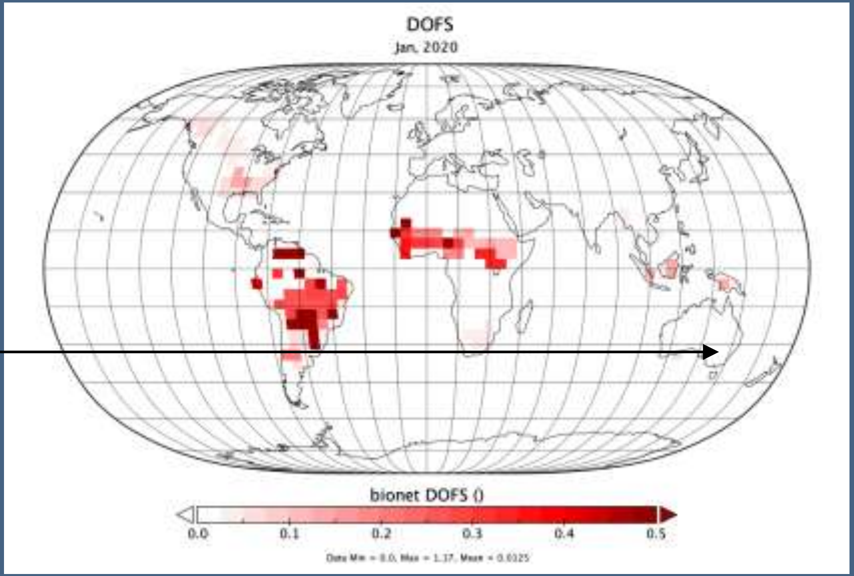




- Information content from OCO-2 for 2015
  - DOFS L0 = 33, L1 = 69, L2 = 134, total DOFS = 675
- Remarkably, Indonesia (Kalamantin) is resolvable in Sept. 2015.
- The dofs indicates that there is information in South America, Northern Africa, and Southeast Asia
- However, there is not information in Southern Africa

The inferno of 2020





- Australia suffered one of its worse biomass burning episodes in recent history.
- However, OCO-2 does not provide a strong constraint in Southeast Australia.

Some subtilities with DOFS calculation—the prior projection

- By approximating the solution $\mathbf{x}_a$ of any χ^2-minimizing inversion (e.g. 4D-var) in our wavelet basis, we can
    1. simulate the inversion in the reduced-dimensional basis,
    2. bound the associated DOFS with high probability.

DOFS of 4D-var

$$\mathrm{Tr}\left(\left(\boxed{\mathbf{C} + \mathbf{\Pi}^{\perp}_{\mathbf{M}^T\tilde{\mathbf{x}}}\mathbf{M}^T\mathbf{B}^{-1}\mathbf{M}\mathbf{\Pi}^{\perp}_{\mathbf{M}^T\tilde{\mathbf{x}}}} + \mathbf{Y}\right)^{-1}\mathbf{Y}\right) \lesssim \boxed{\mathrm{Tr}\left(\mathbf{A}\right)} \lesssim \mathrm{Tr}\left(\left(\lambda\cdot\mathbf{M}^T\tilde{\mathbf{y}}\tilde{\mathbf{y}}^T\mathbf{M} + \mathbf{Y}\right)^{-1}\mathbf{Y}\right)$$

- If we use this as the prior covariance in the reduced-dimensional space, the corresponding low-dimensional inversion retrieves the 4D-var solution with negligible error.
- The posterior covariance and averaging kernel can then be computed analytically, and yield provable bounds on the corresponding quantities for the full-dimensional 4D-var system.

$$\mathbf{A} := (\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}, \text{ (the 4D-var averaging kernel)}$$

$$\mathbf{M} := \text{ Matrix of columnized basis elements for reduced-dimensional space}$$

$$\tilde{\mathbf{x}} := \mathbf{x}_a - \mathbf{x}_b$$

$$\tilde{\mathbf{y}} := \mathbf{H}^T\mathbf{R}^{-1}\left(\mathbf{y} - H(\mathbf{x}_b) - \mathbf{H}\mathbf{M}\mathbf{M}^T\tilde{\mathbf{x}}\right)$$

$$\lambda := \frac{1}{\tilde{\mathbf{y}}^T\mathbf{M}\mathbf{M}^T\left(\tilde{\mathbf{x}}\right)}$$

$$\mathbf{Y} := \mathbf{M}^T\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\mathbf{M}$$

$$\mathbf{\Pi}_{\mathbf{M}^T\tilde{\mathbf{x}}} := \text{Projection onto } \mathbf{M}^T\tilde{\mathbf{x}}$$

$$\mathbf{\Pi}^{\perp}_{\mathbf{M}^T\tilde{\mathbf{x}}} := \text{Projection onto the orthogonal complement of } \mathbf{M}^T\tilde{\mathbf{x}}$$

$$\mathbf{C} := \lambda\cdot\left[\mathbf{\Pi}_{\mathbf{M}^T\tilde{\mathbf{x}}}\mathbf{M}^T\tilde{\mathbf{y}}\tilde{\mathbf{y}}^T\mathbf{M}\mathbf{\Pi}_{\mathbf{M}^T\tilde{\mathbf{x}}} + \mathbf{\Pi}^{\perp}_{\mathbf{M}^T\tilde{\mathbf{x}}}\mathbf{M}^T\tilde{\mathbf{y}}\tilde{\mathbf{y}}^T\mathbf{M}\mathbf{\Pi}_{\mathbf{M}^T\tilde{\mathbf{x}}} + \mathbf{\Pi}_{\mathbf{M}^T\tilde{\mathbf{x}}}\mathbf{M}^T\tilde{\mathbf{y}}\tilde{\mathbf{y}}^T\mathbf{M}\mathbf{\Pi}^{\perp}_{\mathbf{M}^T\tilde{\mathbf{x}}}\right]$$

Conclusions

- Resolution and information content are critical metrics for inverse models and their use, e.g., Global Stocktake.
  - OCO-2 MIP ensembles are crude proxies for resolution
- CMS-MFlux shows that flux resolution—as defined by dofs--enabled by OCO-2 varies substantially in space and time in 4D-var systems.
  - Kalamantin was resolved in Sept, 2015, but not SE Australia in Jan 2020
  - Amazon and north-equatorial Africa can be inferred.
- For 2015, the dofs ~ 675, (~1.5% of all flux grids)
- CMS-MFlux can help interpret the OCO-2 MIP ensemble
  - Currently calculated for 2015-2020 in LNLGOIS