Inverse modelling for trace gas surface flux estimation, impact of a non-diagonal B-matrix

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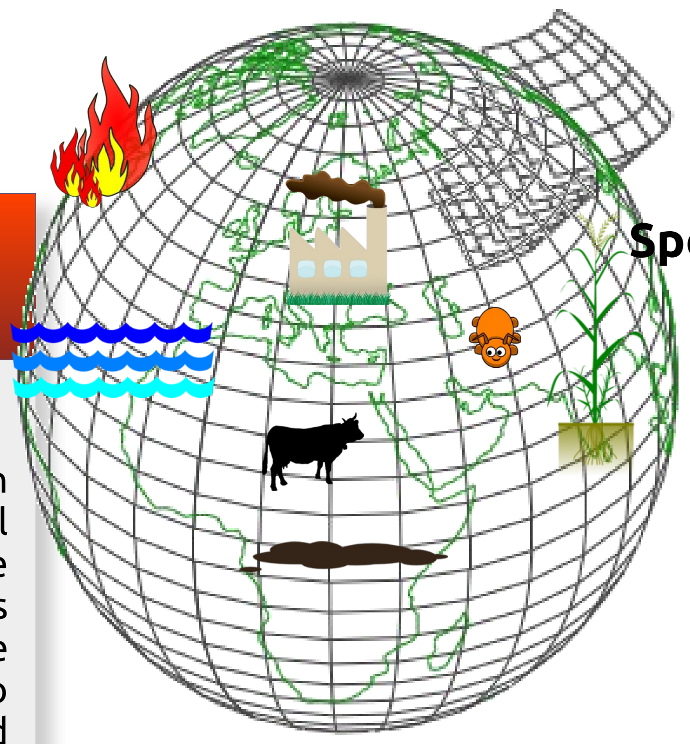

Forward Model: TOMCAT
Species of interest: CH_4
Number of grid points: 64 × 32 × 60 (5⅝° × 5⅝°)
Period: First 100 days of 2018
Chemistry: OH, $O(^1D)$, Cl

$$\frac{\partial \mathbf{x}_t}{\partial t} + \boldsymbol{u} \cdot \nabla \mathbf{x}_t = \mathbf{x}_t^{\mathrm{sf}} + \mathbf{c}$$

CH_4 concentration; Prescribed winds; Surface flux; Chemistry

Inverse Model: INVICAT

$$J(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right) + \frac{1}{2}\left(\mathbf{y}-\mathbf{h}(\mathbf{x})\right)^{\mathrm{T}} \mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{h}(\mathbf{x})\right)$$

Control vector:

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_{t=0}^{\mathrm{ic}} \\ -- \\ \mathbf{x}_{t=0}^{\mathrm{sf}} \\ \mathbf{x}_{t=1}^{\mathrm{sf}} \\ \mathbf{x}_{t=2}^{\mathrm{sf}} \\ \vdots \end{pmatrix}$$

Abstract

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One of the most appealing uses of data assimilation is to infer useful information about a dynamical system that is not observed directly. This is the case for the estimation of surface fluxes of trace gases (like methane). Such fluxes are not easy to measure directly on a global scale, but it is possible to measure the trace gas itself as it is transported around the globe. This is the purpose of INVICAT (the inverse modelling system of the chemical transport model TOMCAT), which has been developed here. INVICAT interprets observations of (e.g.) methane over a time window to estimate the initial conditions (ICs) and surface fluxes (SFs) of the TOMCAT model.

This poster will show how INVICAT has been expanded from a diagonal background error covariance matrix (B-matrix, DB) to allow an efficient representation of a non-diagonal B-matrix (NDB). The results of this process are mixed. A NDB-matrix for the SF field improves the analysis against independent data, but a NDB-matrix for the IC field sometimes appears to degrade the analysis. This poster presents these results and suggests that a possible reason for the degraded analyses is the presence of a possible bias in the system.

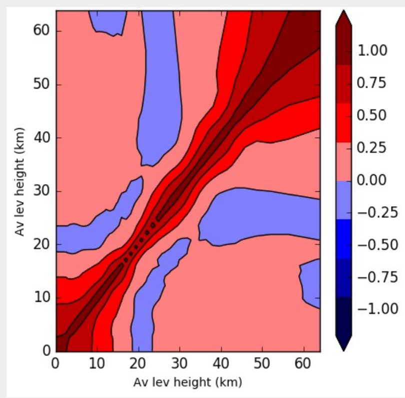
The B-matrix

Configurations tested:

- **For $\mathbf{B}^{\mathrm{ic}}$:**
  - Σ^{ic} = 0.1 × background value
  - Vert. corrs. (see below) on/off
  - Horiz. corrs. (ℓ_{ic}=400 km) on/off
- **For $\mathbf{B}^{\mathrm{sf}}$:**
  - Σ^{sf} = 0.4 × background value
  - Temp. corrs. (τ=2 months) on/off
  - Horiz. corrs. (ℓ_{sf} = 200, 400 km) on/off
  - Horiz. corrs. modelled *explicitly* or *implicitly* (but efficiently) via a *spectral parametrisation*

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}_{t=0}^{\mathrm{ic}} & \vdots & 0 \\ -- & & -- \quad -- \quad -- \\ 0 & \vdots & \mathbf{B}^{\mathrm{sf}} \end{pmatrix}$$

Vertical corr. matrix for $\mathbf{B}^{\mathrm{ic}}$



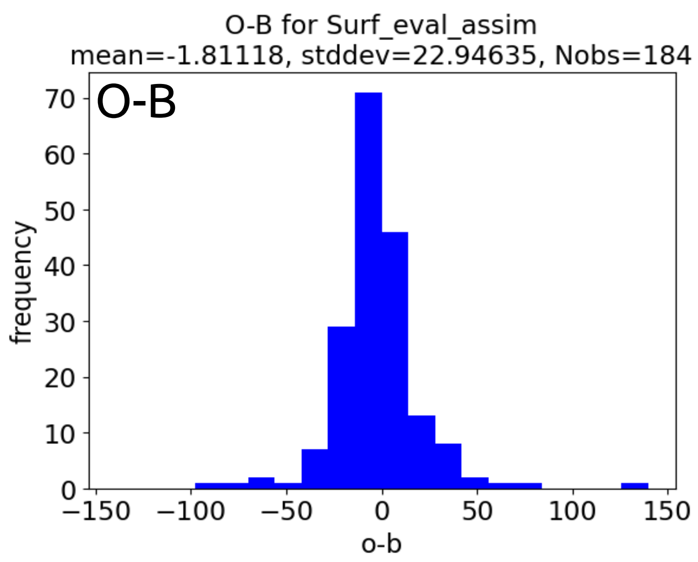
Why use a non-diagonal B-matrix?

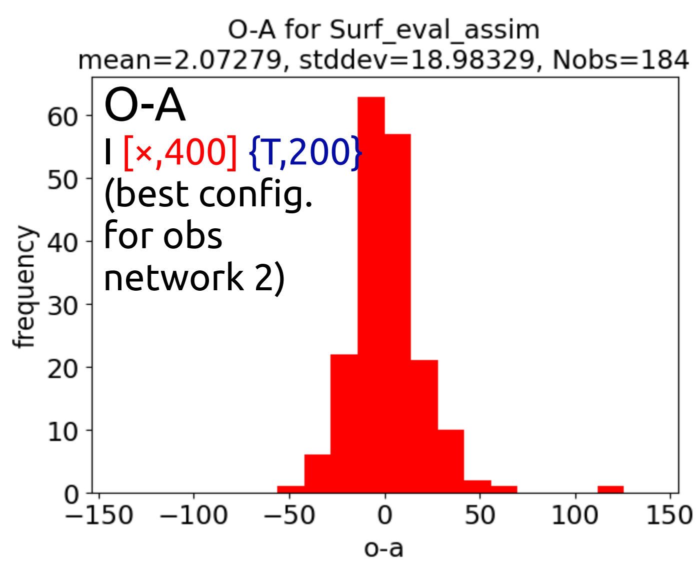
- Diagonal B-matrix:
  - Easy to represent
  - Unrealistic, but potentially well conditioned numerically
  - Lengthscales (ℓ) are the same as the grid boxes
  - Need to know only background error variances
- Non-diagonal B-matrix:
  - Complicated/potentially expensive to represent
  - Need to know:
    - Error variances
    - Horiz. and vert. error corrs. in $\mathbf{x}^{\mathrm{ic}}$
    - Horiz. and temp. error corrs. in $\mathbf{x}^{\mathrm{sf}}$
  - Need to represent a big matrix:
    - Full B: $[(64{\times}32{\times}60) + (64{\times}32{\times}16)]^2 \approx 24 \times 10^9$ elements
    - Horiz. corrs. only (for SF): $[64{\times}32]^2 \approx 4.2 \times 10^6$ elements
  - We test an efficient implicit representation of B via an efficient spectral decomposition method
  - Spectral representation: only 33 elements for horiz!

Experiments

- 665 surface obs.
- ~75% assimilated
- ~25% unassimilated (for evaluation)
- Above chosen randomly three times (obs networks 1, 2, 3)
- Different B-matrix configs. (see key)

Evaluation obs O-B, O-A for obs network 2





Key:

- I/E implicit/explicit representation of B
- Initial concentration part of B
  - [V/×,ℓ/×] = with/without vertical corrs. horiz. lengthscale ℓ km
- Surface flux part of B
  - [T/×,ℓ/×] = with/without temporal corrs. horiz. lengthscale ℓ km ls/~~ls~~ with/without land-sea decoupling (implicit B only)

Standard deviation of O-A for evaluation obs