FINAL REPORT PROGRAM LEFE

Program LEFE/ MANU	Project Title **Assimilation de Données à l'Échelle Régionale : Objectivation des covariances d'erreur et Optimisation de l'utilisation de l'information (ADEROO)**	Years 2020 – 2022

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Contribution to: ICOS[1] ERIC[2], H2020 CHE[3] and VERIFY, Horizon Europe CoCO2[4].

Context

Policy makers need to estimate anthropogenic GHG[5] emissions at the regional scale with operational and cost-effective methods. Today in France, reporting to the UNFCCC[6] is at the yearly national scale. Atmospheric data assimilation may help distributing emissions at the regional scale in an operational framework.

Objectives / scientific questions

The main objective of ADEROO is to design an inversion framework for France to estimate monthly net methane (CH_4) fluxes per region and per activity sector by assimilating atmospheric data from the ICOS network, which could be operational at the yearly national scale.

Main results

The main achievements of ADEROO are methodological and are a continuation of the theoretical work achieved in Berchet et al. (2013) and in a previous GMES-MDD[7] project ESPiGRAD[8] (Pison et al., 2016) on the automatic design of error covariance matrices in atmospheric inversions. The full processing chain of ADEROO is described in Ill. 1 and the new results obtained include:

- the implementation of non-diagonal error statistics matrices in the log-likelihood estimator for analytical inversions
- the optimization of computing time (divided by 10) and the explicit computation of the gradient and Hessian of the likelihood function
- the automation of the analytical inversion scheme by linking it to the Community Inversion Framework (Berchet et al., 2021) and its integration in a python module.

The main scientific results from ADEROO are insights on how to set-up the inversion framework for France. The first set of results consists in information on error correlations:

- the temporal correlations for lateral boundary conditions are large
- the temporal correlations for emissions are about 2 weeks
- there is an anti-correlation between SNAP[9] so that the inversions redistribute the total fluxes among the various activity sectors.
- there is almost no spatial error correlations between the ICOS stations

When using several possible set-ups i.e. with or without correlations in the error statistics matrices combined to defining the control vector by SNAP or by region, the results of the inversions remain consistent (Ill. 2).

References:

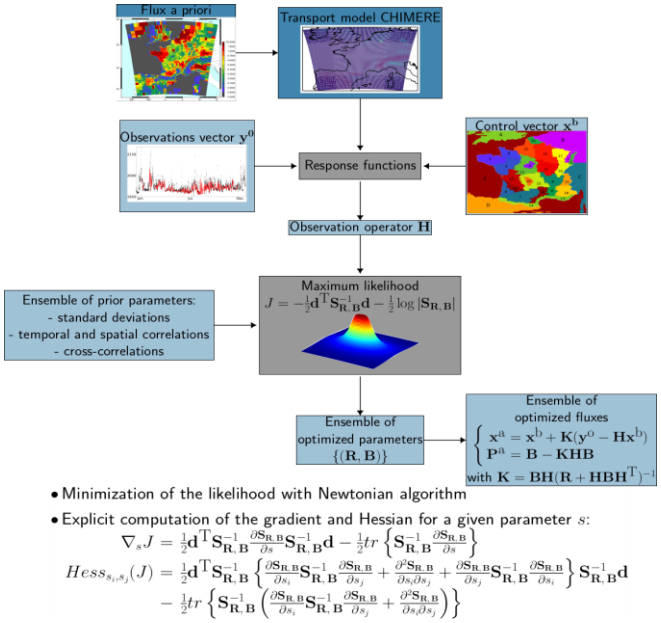
- Berchet, A., Pison, I., Chevallier, F., Bousquet, P., Bonne, J.-L., and Paris, J.-D.: Objectified quantification of

1 Intergrated Carbon Observatory System
2 European Research Infrastructure Consortium
3 CO2 Human Emissions, https://www.che-project.eu/
4 Prototype system for a Copernicus CO2 emission monitoring service, https://coco2-project.eu/
5 GreenHouse Gas
6 United Nations Framework Convention on Climate Change
7 Programme Global Monitoring for Environment and Security du Ministère du Développement Durable
8 Estimation des Sources et Puits de Gaz à effet de serre - CO_2, CH_4 et N_2O - à l'échelle Régionale par Assimilation de Données atmosphériques in-situ
9 Selected Nomenclature for Air Pollution

uncertainties in Bayesian atmospheric inversions, Geosci. Model Dev., 8, 1525–1546, https://doi.org/10.5194/gmd-8-1525-2015, 2015.

- Pison, I., Berchet, A., Saunois, M., Bousquet, P., Broquet, G., Conil, S., Delmotte, M., Ganesan, A., Laurent, O., Martin, D., O'Doherty, S., Ramonet, M., Spain, T. G., Vermeulen, A., and Yver Kwok, C.: How a European network may help with estimating methane emissions on the French national scale, Atmos. Chem. Phys., 18, 3779–3798, https://doi.org/10.5194/acp-18-3779-2018, 2018.
- Berchet, A., Sollum, E., Thompson, R. L., Pison, I., Thanwerdas, J., Broquet, G., Chevallier, F., Aalto, T., Berchet, A., Bergamaschi, P., Brunner, D., Engelen, R., Fortems-Cheiney, A., Gerbig, C., Groot Zwaaftink, C. D., Haussaire, J.-M., Henne, S., Houweling, S., Karstens, U., Kutsch, W. L., Luijkx, I. T., Monteil, G., Palmer, P. I., van Peet, J. C. A., Peters, W., Peylin, P., Potier, E., Rödenbeck, C., Saunois, M., Scholze, M., Tsuruta, A., and Zhao, Y.: The Community Inversion Framework v1.0: a unified system for atmospheric inversion studies, Geosci. Model Dev., 14, 5331–5354, https://doi.org/10.5194/gmd-14-5331-2021, 2021.

Illustration 1



- Minimization of the likelihood with Newtonian algorithm
- Explicit computation of the gradient and Hessian for a given parameter s:

$$\nabla_s J = \frac{1}{2}\mathbf{d}^{\mathrm{T}}\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s}\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\mathbf{d} - \frac{1}{2}tr\left\{\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s}\right\}$$

$$Hess_{s_i,s_j}(J) = \frac{1}{2}\mathbf{d}^{\mathrm{T}}\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\left\{\frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_i}\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_j} + \frac{\partial^2 \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_i \partial s_j} + \frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_j}\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_i}\right\}\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\mathbf{d} - \frac{1}{2}tr\left\{\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\left(\frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_i}\mathbf{S}_{\mathbf{R},\mathbf{B}}^{-1}\frac{\partial \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_j} + \frac{\partial^2 \mathbf{S}_{\mathbf{R},\mathbf{B}}}{\partial s_i \partial s_j}\right)\right\}$$

Illustration 2

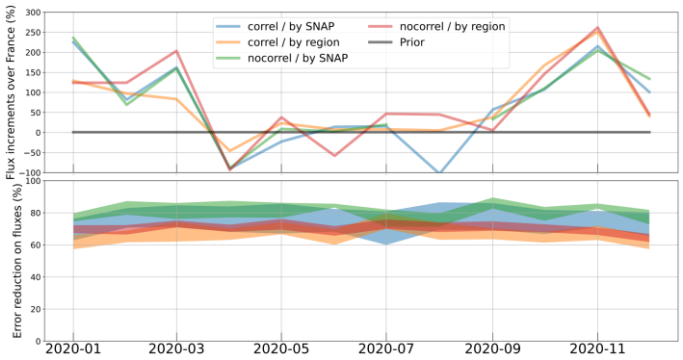


Illustration 1: full ADEROO processing chain to automatically generate error statistics in the framework of analytical greenhouse gas inversions in France. In ADEROO, the processing chain was optimized and now allows non diagonal matrices, hence accommodating spatial and temporal correlations in the system, contrary to previous work.

Illustration 2: retrieved monthly fluxes for 2020 for various set-ups, including or not correlations.

Future of the project :

Scientific perspectives:

- further assess the impact of error correlations at the monthly and regional scales
- propagate the method to more recent years and systematically deploy the system for French national inversions
- use machine-learning to infer unstructured covariance matrices accounting for complex atmospheric patterns

Number of publications, communications and theses

- Poster presentation at the annual LEFE symposium in Toulouse in June 2023
- Insights from ADEROO will be aggregated and finalized to produce a scientific publication

Data availablility

The project is based on the Community Inversion Framework available at doi: 10.5281/zenodo.6304912