GC31B-1169

Developing a high-resolution CO_2 flux inversion model for global and regional scale studies

Shamil Maksyutov [1], Rajesh Janardanan[1], Makoto Saito[1], Akihiko Ito[1], Tom Oda[2], Johannes W Kaiser[3], Dmitry Belikov[1,4], Alexander Ganshin[5] , Vinu Valsala[6], Motoki Sasakawa[1] and Toshinobu Machida[1]

(1) National Institute for Environmental Studies, Tsukuba, Japan (shamil@nies.go.jp),
(2) USRA, GSFC, NASA, Greenbelt, MD, USA
(3) Max Plank Institute for Chemistry, Mainz, Germany
(4) National Institute for Polar Research, Tokyo, Japan
(5)Central Aerological Observatory, Dolgoprudny/Tomsk State Univ. , Tomsk, Russia
(6)Indian Institute for Tropical Meteorology, Pune, India

Abstract We develop and test an iterative inversion framework that is designed for estimating surface CO_2 fluxes at a high spatial resolution using a Lagrangian-Eulerian coupled tracer transport model and atmospheric CO_2 data collected by the global in-situ network and satellite observations. In our inverse modeling system, we employ the Lagrangian particle dispersion model FLEXPART that was coupled to the Eulerian atmospheric tracer transport model (NIES-TM). We also derived an adjoint of the coupled model. Weekly corrections to prior fluxes are calculated at a spatial resolution of the FLEXPART-simulated surface flux responses (0.1 degree). To obtain a best fit to the observations we tested a set of optimization algorithms, including quasi-Newtonian algorithms and implicitly restarted Lanczos method. The square root of covariance matrix for surface fluxes is implemented as implicit diffusion operator, while the adjoint of it is derived using automatic code differentiation tool. The model was applied to assimilating one year of Obspack data, and produced satisfactory flux correction results. Regional version of the model was applied to inverse model analysis of the CO_2 flux distribution in West Siberia using continuous CO_2 observation data by tower observation network JR-Station.

For simulation of the CO_2 transport in the atmosphere we use a coupled Eulerian-Lagrangian model NIES-TM – Flexpart, which combines NIES TM v08.1i (resolutions of 2.5, 5, 10 degree and 32 vertical levels), (Belikov et al, 2013) and Flexpart model (Stohl, 2005), with surface flux resolutions of 0.1, 0.2, 1.0 degree and daily flux data. For application to grid based inversion, a manually developed adjoint of the NIES TM v08.1i was completed. Transpose of the receptor sensitivity matrixes simulated by Flexpart was simpler to implement. Accuracy of NIES TM adjoint was found to be 1e-9, while for receptor sensitivity matrixes simulated by Flexpart it is 1e-16 (double precision is used normally).

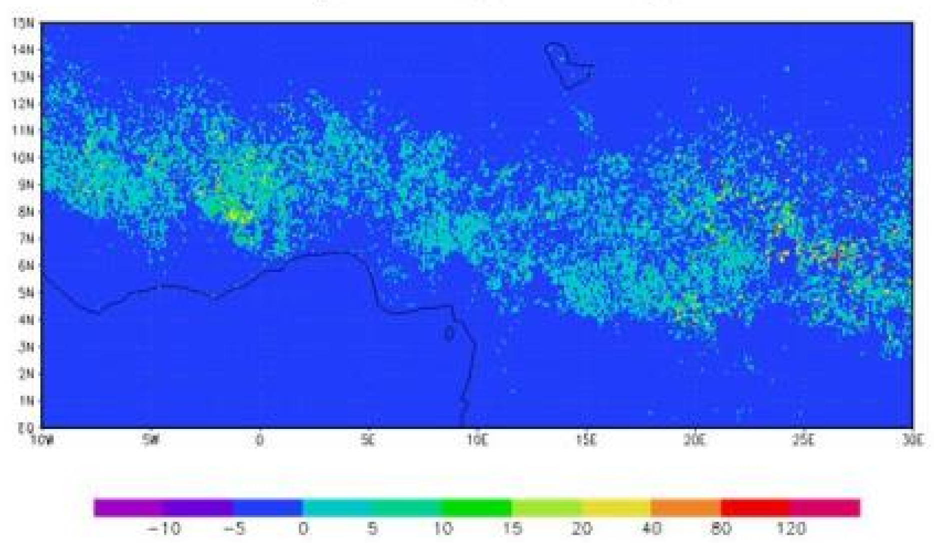
-Configuration of NIES-TM
- flexible resolution (2.5 or 5 or 10 degree), use low resolution of 10x10 degree for faster convergence in the tests
- reduced grid, larger longitudinal grid size near poles (Belikov 2013)
- mass conserving meteorology, mass fluxes on hybrid isentropic vertical coordinates interpolated from JCDAS
- hand-coded adjoint with same CPU cost in forward and adjoint modes

Configuration of Flexpart
- -JCDAS meteorology (1.25 deg, 40 model levels, 6 hourly)
- -flux footprints estimated on 0.1x0.1 deg grid, hourly time step
- -time window 2 to 3 days (for coupling to NIES-TM at 0 GMT)
- -for coupling to NIES-TM, initial concentration footprints estimated on isentropic vertical grid at 2.5 deg horizontal resolution

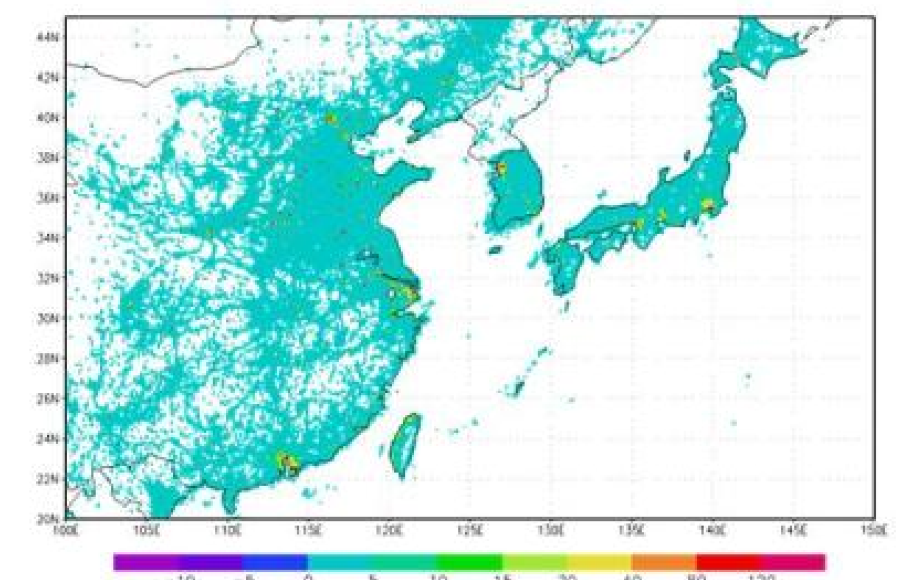
Prior fluxes for high resolution (0.1 deg) transport simulation
-Fossil fuel emissions
  -ODIAC 1 km monthly fluxes aggregated to 0.1 degree
-Terrestrial biosphere
  -VISIT NEE simulation with JCDAS meteorology, 0.5 deg grid, interpolated to 0.1 deg, using MODIS 1km land/ocean mask.
-Forest fire
  -GFAS daily at 0.1 degree
-Ocean sink
  -OTTM monthly 1x1 deg fluxes interpolated to 0.1 deg, using MODIS 1km land/ocean mask
-Land/ocean uncertainties
  - Monthly mean of VISIT GPP simulation with CFSR meteorology, ~0.3 deg Gaussian grid, interpolated to 0.1 deg
  - OTTM monthly 1x1 deg flux variance, with min 0.02 gC/m2/day interpolated to 0.1 deg, using MODIS 1km land/ocean mask

-Observational data: Obspack dataset globally and daytime JR-STATION data in West Siberia.
-Analysis period 48 'weeks' Jan 1, 2010 –Dec 31,2010. Week defined as ¼ of a month
-Optimization problem: reconstruct fluxes and uncertainties at weekly time step at resolutions up to 0.1 deg (results with 0.1 deg presented, tests done also with 0.2 deg and 1 deg) Target: estimate flux singular vectors, uncertainty, uncertainty reduction
-Technical data
 - size of lagrangian H matrix 30 GB/year for surface, 146 GB/year for GOSAT
 -Performance:
 -Most of CPU time spent on FLEXPART calculation, done in parallel on 96 cores
 -Estimation of 40 singular vectors requires 80 vector multiplications by A^TA or AA^T, takes 6 hours on 4 cores

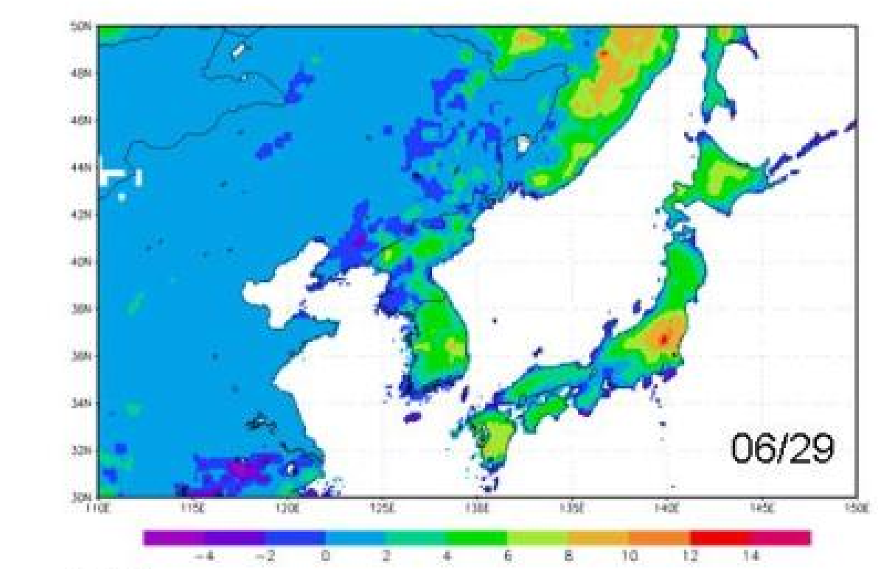
Prior CO_2 fluxes (gC/m^2/day)



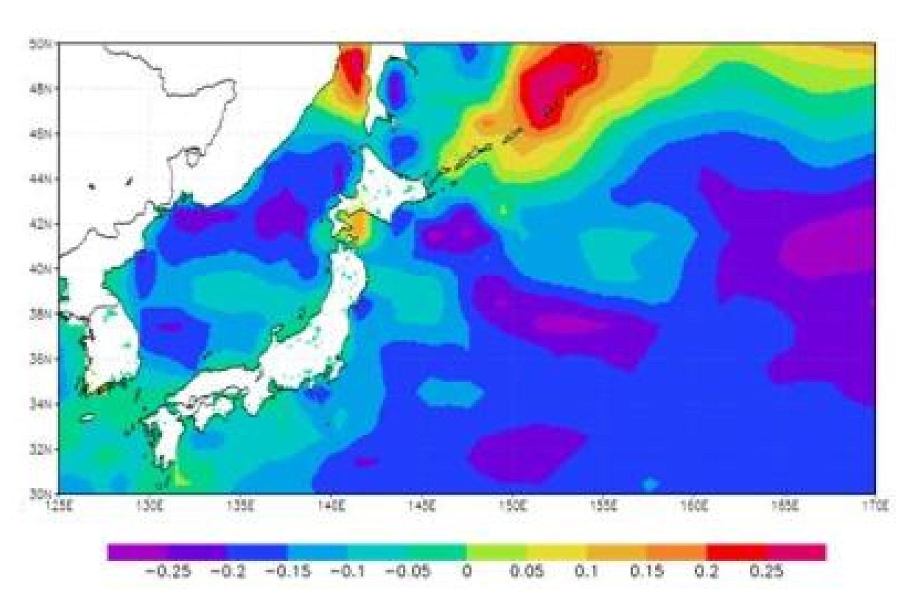
Africa: Forest fire by GFAS (Kaiser et al), Jan



E Asia fossil emissions ODIAC, Jan



Daily terrestrial ecosystem fluxes by VISIT



OTTM ocean flux, Jan

Inverse problem $\quad y = H \cdot (x_p + x)$

y – CO_2 observations by GOSAT, H – transport model, x_p – prior flux
x – grid-resolving flux correction field

As the problem is ill-constrained in case of large dimension of x, regularization is applied by optimizing cost function

$$J = \frac{1}{2}(r - H \cdot x)^T R^{-1} (r - H \cdot x) + \frac{1}{2} x^T B^{-1} x$$

$r = y - H \cdot x_p$ is residual misfit of forward simulation

B provides smoothing constraint on x, (flux uncertainty)

R is covariance for data-model mismatch (data uncertainty)

In atmosphere/ocean data assimilation algorithms, eg (Fisher and Courtier, 1995), square root of B is used to simplify the problem $\quad B = L \cdot L^T$

With L known, optimization problem can be reduced by applying substitutions:

$$x = L \cdot z \qquad R = \sigma \cdot \sigma^T \qquad b = \sigma^{-1} r \qquad A = \sigma^{-1} H \cdot L$$

New form of cost function: $\quad J = \frac{1}{2}(b - A \cdot z)^T (b - A \cdot z) + \frac{1}{2} z^T z$

The solution minimizing J is obtained by forcing derivative J' to 0:

$\partial J / \partial z = A^T (A \cdot z - b) + z = 0$ which leads to $z = (A^T A + I)^{-1} A^T b$

Meirink, ACP, 2008 and Basu, ACP, 2013 used SVD algorithm by Lanczos 1950 to solve this equation

Covariance matrix construction. Factorization of L

History: Matrix B and its square root L were first derived in 2-D spline theory, then applied to data assimilation in both 3-D var and 4-D var.
Dimension of problem requires applications of most memory efficient algorithms, which is similar to high resolution ocean/atmosphere assimilation problems. In ocean modeling the Gaussian shape representation is simulated by applying horizontal diffusion operator (Weaver and Courtier, QJRMS, 2001). We use method of alternating dimensions to split implicit diffusion operator in to lat and lon directions.

Following Meirink ACP 2008 we use factorization of L by directions: $L = L_t \otimes L_y \otimes L_x \otimes u_x$, (where $\otimes$ is Kroneker product) with the L matrixes in directions of lon, lat and time, and u_x is flux uncertainty on 0.1x0.1 grid.
This factorization is easy to implement when land and ocean fluxes each are treated separately as global fields (Basu et al, 2013).

Solvers: truncated SVD and LBFGS

As dimension of A is too big, we use truncated SVD of A to find solution:

SVD of A, $A = U \Sigma V^T$ found by applying Lanczos process to AA^T giving singular vectors U, V and singular values Σ. Once SVD decomposition is known, the solution is found by transforming the variables to SV vector space (Rayner et al, Tellus, 1999) and back:

$$s = V^T z \quad , \quad d = U^T b \qquad \text{resulting in} \qquad s = \frac{\Sigma^T d}{\Sigma^T \Sigma + I}$$

which is solved easily as matrix Σ is diagonal.

The expression for flux x follows as $\quad x = LV \frac{\Sigma^T U^T b}{\Sigma^T \Sigma + I}$

The posterior flux uncertainty is also available as: $\quad B_{post} = L \cdot V \frac{I}{\Sigma^T \Sigma + I} (L \cdot V)^T$

Alternatively, application of LBFGS to minimization appears computationally more efficient, but without explicit estimate of posterior covariance matrix

Flux estimates over West Siberia using West Siberian JR-STATION data

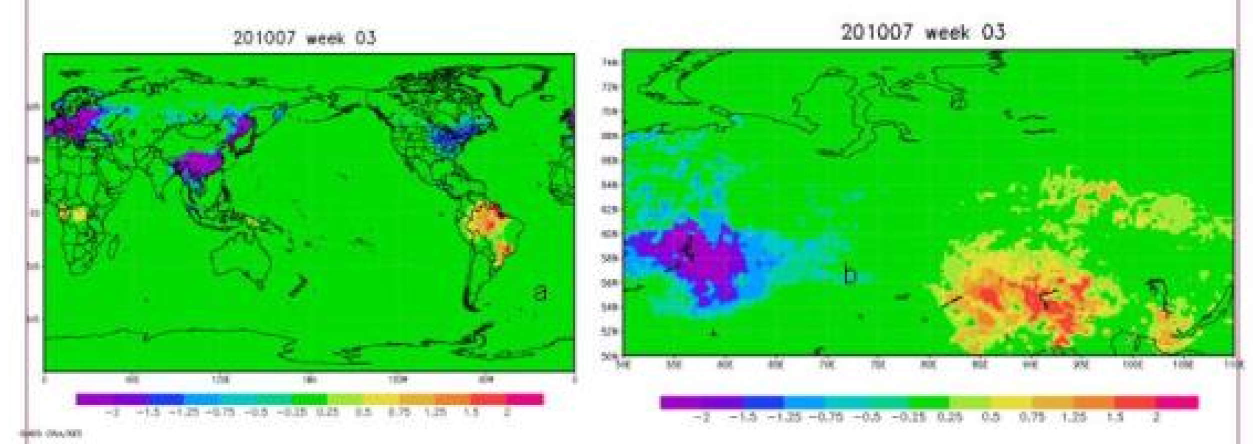
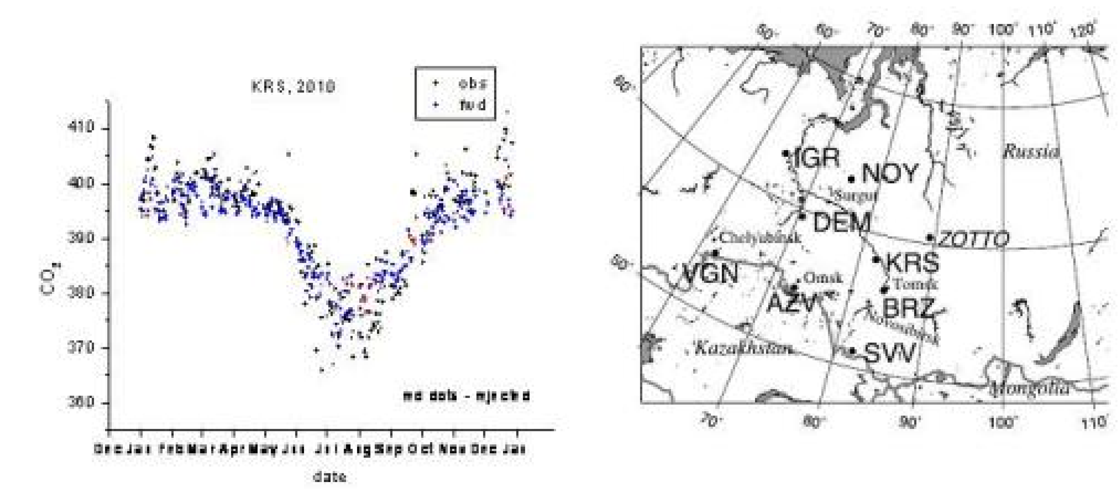


Fig.1 Global flux increments due to use of Obspack data (a) and flux corrections over West Siberia (b) due to addition of the West Siberian JR-STATION data

Fig. 2 Forward model simulation at Karasevoe



SUMMARY

We demonstrated technical feasibility of computationally efficient approach for retrieving fine-grid scale information using surface observations.

The model can be used for forward simulation and estimating surface CO_2 fluxes at variable resolution from 1.0 to 0.1 deg

Further improvement of the technique is needed, including:
-Developing higher resolution wind data for GOSAT period, using NICAM nudged simulation at 28 km resolution combined with Flexpart –
-Increasing number of estimated singular vectors (apply restarted mode)
-Preparing very high resolution biopsheric fluxes and flux uncertaities using MODIS GPP and vegetation index products at 5 km and 1 km resolution

References

Basu, S., Guerlet, S., Butz, A., Houweling, S., et al.: Atmos. Chem. Phys., 13, 8695-8717, doi:10.5194/acp-13-8695-2013, 2013.
Belikov, D. A., Maksyutov, S., Sherlock, V., Aoki, S.et al: Atmos. Chem. Phys., 13, 1713-1732, 2013
Belikov, D. A., Maksyutov, S., Yaremchuk, A., Ganshin, A., Kaminski, T., Blessing, S., Sasakawa, M., and Starchenko, A., Geosci. Model Dev. Discuss., 8, 5983-6019, doi:10.5194/gmdd-8-5983-2015, 2015.
Fisher, M. and Courtier, P: ECMWF Tech. Memo. 220 , 1995.
Hansen P. C. The truncated SVD as a method for regularization, BIT Numerical Mathematics, 27, 4, 534-553, 1987
Lanczos C. An iteration method for the solution of the eigenvalues problem of linear differential and integral operators", J. Res. Nat. Bur. Stand, v. 45, 255-282, 1950
Maksyutov S., Y. Nakatsuka, V. Valsala, M. Saito, et al: Algorithms for carbon flux estimation using GOSAT observational data. CGER's supercomputer monograph report, 15, CGER-I092-2010, 112 pp, 2010
Maksyutov, S., Takagi, H., Valsala, V. K., Saito, et al:Atmos. Chem. Phys., 13, 9351-9373, doi:10.5194/acp-13-9351-2013, 2013.
Meirink, J. F., Bergamaschi, P., and Krol, M. C.: Atmos. Chem. Phys. Discuss., 8, 12023-12052, doi:10.5194/acpd-8-12023-2008, 2008.
Nocedal J., : Mathematics of Computation 35, 773-782, 1980.
Rödenbeck, C. : MPI BGC, Jena, Technical report n.6, ISSN 1615-7400, 2005
Stohl, A., C. Forster, A. Frank, P. Seibert et al: Atmos. Chem. Phys. 5, 2461-2474, 2005
Weaver, A. and Courtier, P.: Q.J.R. Meteorol. Soc., 127: 1815–1846, 2001
Wu K. and H. Simon: . SIAM Journal on Matrix Analysis and Applications, 22, 2, 602-616, 2001.