Development of adjoint of the coupled Eulerian-Lagrangian transport model for CO₂ inverse modeling in the subarctic

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The arctic and subarctic regions are large carbon reservoirs. Permafrost soils covering about 25% of the land surface in the Northern Hemisphere store almost twice as much carbon as is currently present in the atmosphere. Schuur et al. (2009) found that areas which thawed over the past 15 years had 40% greater annual losses of old carbon than minimally thawed areas, while areas that thawed decades earlier lost even more old carbon (78% greater than minimally thawed areas). Organic carbon in permafrost soils could act as a positive feedback to global climate change due to enhanced biospheric respiration rates with warming. The comparison of observation performed in 1958-61 and 2009-11 reveals a strikingly large (~50%) amplitude increase north of 45°N, which must be attributed almost entirely to the terrestrial biosphere (Graven et al., 2013). None of the considered terrestrial ecosystem models currently participating in the fifth phase of the Coupled Model Intercomparison Project (CMIP5) can account for the increase in CO2 amplitude. However, there is a high degree of uncertainty regarding the rate of carbon release due to permafrost thaw, and the microbial decomposition of previously frozen organic carbon and the terrestrial biosphere activity. Moreover, the scarcity of observations in the subarctic means that the carbon cycle there is not well monitored.

During the last decades an observational network of increasing density is being established, measurements on board of ships and airplanes as well as space-borne observations are also becoming available to monitor the greenhouse gases in the atmosphere. Hence such observations provide a possibility to estimate their sources and sinks in more regions. In order to link the surface fluxes to the atmospheric concentration observations, an accurate model of the atmospheric transport and inverse modeling technique are needed. A number of studies have addressed improvements to the inverse methods of the atmospheric transport. The challenging task is using the information from a spatially sparse observational network in an optimal way to derive regional flux estimates together with an estimated range of confidence.

CO2 is a long-lived species as result the transport model has to cover a long simulation period to relate fluxes and concentrations. Therefore, computing time is a critical issue, and methods have been developed to optimize it. In case of a chemically inert tracer, the simulated concentration at observational locations is linear, and thus the transport can be represented by the model's Jacobian matrix. Usually such a matrix has been computed by multiple runs of a transport model for a set of prescribed surface flux patterns. The adjoint of transport model allows the efficient evaluation of derivatives of the simulated tracer concentration at observational locations with respect to the tracer's sources and sinks (Kaminski et al., 1999). The adjoint approach appeared in the field of atmospheric science in the early 1970s first time and came to be applied extensively in meteorology later. In the 1990s the method has expanded to include ever more detailed CTMs (Kaminski et al., 1999).

Here we present a development of an inverse modeling system employing an adjoint of National Institute for Environmental Studies (NIES) three-dimensional transport model (TM) coupled with a Lagrangian plume diffusion model. The adjoint has been constructed automatically in the "reverse mode" of automatic differentiation by means of the Transformation of Algorithms in Fortran (TAF) software (http://www.FastOpt.com).

NIES TM is a three-dimensional atmospheric transport model, which solves the continuity equation for a number of atmospheric tracers on a grid spanning the entire globe. Spatial discretization is based on a reduced latitude-longitude grid and a hybrid sigma-isentropic coordinate in the vertical. NIES TM uses a horizontal resolution of 2.5°×2.5° (Belikov et al., 2013a,b). To resolve synoptic-scale tracer distributions and to have the ability to optimize fluxes at resolutions of 0.5° and higher we coupled NIES TM with the Lagrangian model FLEXPART (version 8.0; Stohl et al., 2005). The Lagrangian component of the forward and adjoint models uses precalculated responses of the observed concentration to the surface fluxes and 3-D concentrations field simulated with the FLEXPART model. NIES TM and FLEXPART are driven by JRA-25/JCDAS reanalysis dataset, with PBL heights provided by ERA interim reanalysis.

The discrete adjoint obtained through automatic differentiation using TAF software is validated via comparison of adjoint gradients to forward model sensitivities calculated using the finite difference approximation (Henze at al., 2007). Forward model sensitivity is calculated using the one-sided finite difference equation.

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A significant amount of computation can be saved by isolating the transport equations. In this approach, the NIES TM is used to produce a frozen archive of atmospheric mass fluxes, which is then used by an "offline" model dedicated to passive transport. The time step of the mass flux archive is usually about a few hours (typically 6) and intermediate fluxes are deduced by interpolation. To speed up calculation we use Message Passing Interface (MPI) parallelization with the model domain decomposition. The computational cost of the adjoint (backward only) of the coupled model is only two times more that of the forward model.

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References

Belikov, D. A., S. Maksyutov, M. Krol, a. Fraser, M. Rigby, H. Bian, a. Agusti-Panareda, D. Bergmann, P. Bousquet, P. Cameron-Smith, M. P. Chipperfield, a. Fortems-Cheiney, E. Gloor, K. Haynes, P. Hess, S. Houweling, S. R. Kawa, R. M. Law, Z. Loh, L. Meng, P. I. Palmer, P. K. Patra, R. G. Prinn, R. Saito, and C. Wilson, Off-line algorithm for calculation of vertical tracer transport in the troposphere due to deep convection, Atmos. Chem. Phys., 13, 1093–1114, doi:10.5194/acp-13-1093-2013, 2013a.

Belikov, D. A., S. Maksyutov, V. Sherlock, S. Aoki, N. M. Deutscher, S. Dohe, D. Griffith, E. Kyro, I. Morino, T. Nakazawa, J. Notholt, M. Rettinger, M. Schneider, R. Sussmann, G. C. Toon, P. O. Wennberg, and D. Wunch, Simulations of column-average CO2 and CH4 using the NIES TM with a hybrid sigma–isentropic (σ – θ) vertical coordinate, Atmos. Chem. Phys., 13, 1713-1732, doi:10.5194/acp-13-1713-2013, 2013b.

Graven, H. D., R. F. Keeling, S. C. Piper, P. K. Patra, B. B. Stephens, S. C. Wofsy, L. R. Welp, C. Sweeney, P. P. Tans, J. J. Kelley, B. C. Daube, E. A. Kort, G. W. Santoni, and J. D. Bent, Enhanced Seasonal Exchange of CO2 by Northern Ecosystems Since 1960, Science, 1239207, DOI:10.1126/science.1239207, 2013.

Henze, D. K., Hakami, A., and Seinfeld, J. H.: Development of the adjoint of GEOS-Chem, Atmos. Chem. Phys., 7, 2413-2433, doi:10.5194/acp-7-2413-2007, 2007.

Kaminski, T., M. Heimann, and R. Giering, A coarse grid three-dimensional global inverse model of the atmospheric transport:1. Adjoint model and Jacobian matrix, J. Geophys. Res., 104(D15), 18,535–18,553, doi:10.1029/1999JD900147, 1999.

Schuur, E. A. G., J. G. Vogel, K. G. Crummer, H. Lee, J. O. Sickman, and T. E. Osterkamp., The effect of permafrost thaw on old carbon release and net carbon exchange from tundra, Nature 459, 556–559, 2009.

Stohl, A., Forster, C., Frank, A., Seibert, P., and Wotawa, G.: Technical note: The Lagrangian particle dispersion model FLEXPART version 6.2, Atmos. Chem. Phys., 5, 2461–2474, doi:10.5194/acp-5-2461-2005, 2005.