Inverse modeling of surface emissions for local pollution:
A new methodology applied to academic test cases
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- **Needs:** Optimize surface emissions using daily recorded ozone and NOX surface concentrations

- **Methodology:** develop an inverse model based on the CTM chimere, including a non-linear optimizer and the adjoint model

- **Test cases:**
  - academic cases to test and improve the methodology
  - real cases of summertime pollution events over the Paris area (based on the ESQUIF IOP’s of July and August, 1998 and 1999)

- Work done in the framework of the OPTEMI project financed by PRIMEQUAL2, program of the french ministry of environment

First-guess emissions inventory for the Paris area, provided by the AIRPARIF network and used in CHIMERE
(1) Numerical approach

- **Input**: a surface emission inventory (first-guess) and meteorological fields (supposed known)

- **Searched outputs**: correction coefficients for emitted species at each time and each surface flux

- **Direct simulation**: from input parameters, modeled concentrations are estimated and compared to measurements

- **Adjoint simulation**: for selected output concentrations, sensitivity to all input parameters is estimated

- **Coupling the two** with a nonlinear optimizer (INRIA N1QN3) makes it possible to update surface emissions in order to better model concentrations fields.
(2) Numerical approach

- The problem of minimization applied to “local pollution problems”: Contrarily to global, tropo-strato inverse modeling studies: local pollution is very under-constrained problem:
  - with large variations in time: one order of magnitude between background traffic emissions and rush-hour peaks and an important spatial heterogeneity of emissions
  - with a very complex urban meteorology within the boundary layer
  - with chemical regimes, pollution concentrated plumes leading to high horizontal gradients etc.

- Only a few constraints (surface measurements): ~ 5-10% of the whole studied domain, with an unknown representativity

*Ozone correlation between aircraft measurements and chimere simulations*

*Calculation of systematic biases between NO modeled and measured concentrations: more important at the traffic peak time.*
The background matrix representing variance/covariance errors on first-guess is unknown. Contrarily to global studies, there is no way to estimate and update it at the local scale in urbanized areas.

The background matrix for emissions is replaced by an increased number of constraints on the concentrations. Cost function reduced to: \( J=(y-x)^T R (y-x) \)

where \( y \) are the measurements concentrations, \( x \) the modeled concentrations and \( R \) the observations matrix.

The new constraints are issued from kriging, an approach similar to optimal interpolation, see examples on the right:
- top: original simulation
- bottom: same ozone fields after analysis
The new approach is tested on academic test cases designed as:

- An academic meteorology considered as the reality
- Academic emissions considered as reality are used to generate the “real” observations
- Perturbed emissions are used for a direct simulation considered as the “first-guess”

The capability of the method is estimated by the differences between “real” and “optimized” emissions and “observations” and “modelled” surface concentrations.

Emissions are perturbed during the whole simulation and optimized between hours 08:00 (32) and 14:00 (38). The goal is to retrieve the 1.2 coeff. representing the distance between “reality” and “first-guess”.

Urban [O3] concentrations are improved within the optimization interval.