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Nudging technique for scale bridging in air quality/climate atmospheric composition modelling

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Abstract

The interaction between air quality and climate involves dynamical scales that cover an immensely wide range. Bridging these scales in numerical simulations is fundamental in studies devoted to megacity/hot-spot impacts on climate. The nudging technique is proposed as a bridging method that can couple different models at different scales.

Here, nudging is used to force low resolution chemical composition models using a high resolution run on critical areas. A one-year numerical experiment focused on the Po Valley hot spot is performed using the BOLCHEM model to asses the method.

The results show that the model response is stable to perturbation induced by the nudging and that, if a high resolution run is taken as a reference, there is an increase in model skills of low resolution run when the technique is applied. This improvement depends on the species and the season. The effect spreads outside the forcing area and remains noticeable over an extension about 9 times larger.

1 Introduction

Processes determining the atmospheric composition cover a wide spectrum of scales, ranging from the global, relevant for climate and large scale transport episodes, like volcanic eruptions or large forest fires, to molecular, where dissipation of energy takes place along with the basic transformation processes (chemical reactions and removal).

Studying the interaction between climate and anthropogenic activities, especially those concentrated in megacities/hot-spots, requires the description of interacting processes on a wide variety of scales, from those typical of anthropogenic emissions, to the global scale.

The simultaneous explicit description of processes at very different scales is limited by computer resources. Therefore, the need to allow different scales to interact calls for a variety of approaches to bridge them.

This connection is already well established in the direction of global-to-regional (or regional-to-local), since it is the result of using output from coarser models to feed boundary conditions into more refined (and limited area) models. This one-way nesting approach is routinely used in atmospheric modelling including meteorological applications (Mass et al., 2002) and, more recently, atmospheric composition studies and forecast applications (Huijnen et al., 2010).

The exchange of information in the reverse direction is highly problematic though of great interest. In fact, uncertainties in large scale simulations are expected to derive a large contribution from the most polluted areas. Here the highly inhomogeneous distribution of sources and the intrinsic non-linearity of the processes involved may give rise to significant departures from fine scale simulations.

Different methods have been used so far to provide better descriptions in specific locations. Certainly the most used, at least with regard to atmospheric dynamics, is the two-way nesting, where one or more subdomains are covered by a grid of resolution finer than the parent simulation. The fine scale simulation communicates with the parent taking boundary conditions as forcing, and giving back fields resulting from some averages over the fine grid. The two-way nesting generally performs better than the one-way nesting (Harris and Durran, 2010), but the former is more difficult to implement and is seldom used (Misenis and Zhang, 2010; Moeng et al., 2007)

Other models adopt stretched grids (Struzewska and Kaminski, 2008; de Meij et al., 2009), where a single grid with variable horizontal resolution permits focusing on a selected area. This approach has the advantage that there are no duplicate runs with different resolutions and the information can propagate in a natural way across the scales. On the other hand, the drawback is that with this approach refining resolution in the area of interest also implies refinement in other areas. More important from a scientific point of view, this approach does not usually take into account different parameterisations for different resolutions.

Actually, when looking at the air quality/climate interactions, processes accounting for different scales are so different that they cannot be dealt with using one model only.

Bridging those scales is much more a matter of coupling different models.

This can be done by forcing a low resolution run using results from a high resolution simulation. Such forcing can be performed using a data assimilation approach. Here, we adopt nudging as the simplest technique of performing the bridging.

The most interesting feature of this technique is that, in contrast with others (two-way nesting, grid stretching, etc.), it can be applied to couple different models. Therefore, it is suitable, for example to force global models using regional or local models, whithout a direct dynamic two-way interaction.

In the approach it is assumed that the high resolution run provides results nearest to the truth. Although this is not always straightforward for the state-of-the-art models and typical resolutions (Valari and Menut, 2008), this assumption relies on the consideration that once the input is known at any resolution, the quality of the solution of a discretised system of equations increases with increasing resolution.

The aim of this paper is to evaluate the effectiveness of such approach. An experiment will be performed using the BOLCHEM (Mircea et al., 2008) model at two different resolutions to simulate a two-model configuration. It must be kept in mind that the real application to the two-model configuration would also present the difficulty of exchanging information between two different chemical mechanisms and two possibly different vertical coordinate systems. Using the same model at two resolutions allows us to isolate the effect of exchanging information, highlighting the effect of non-linearities only.

2 Bridging the scales: the nudging technique

The basic idea of the nudging technique is to force the model run towards available measurements (the "truth") with some relaxation term in the governing equations. The nudging method is widely used in many fields of atmospheric modelling (Haase et al., 2000; Davolio and Buzzi, 2004) and air quality simulations (Kim et al., 2010) to assimilate data into model runs.

In the present application of the nudging concept, the concentration in a certain region of the model domain during a low resolution (LR-N) run is forced to the fields obtained from a high resolution (HR) run which uses a non-forced low resolution (LR) run as boundary conditions.

The technique consists of adding a term to the concentration tendency equation in the model running at low resolution. This term acts to force the computed concentrations towards the high resolution concentrations obtained from a fine scale model. In general the forcing is applied to the low resolution model in the following form:

$$C_{\text{LR-N}}(x,y,z,t+\Delta t) = C_{\text{LR-N}}(x,y,z,t) + \frac{\Delta t}{\tau}\left[C_{\text{HR-r}}(x,y,z,t) - C_{\text{LR-N}}(x,y,z,t)\right] \quad (1)$$

where $C_{\text{HR-r}}$ is the concentration derived fron the HR run and averaged over the LR grid, τ is the relaxation time, which regulates how fast the actual fields are relaxed to the high resolution, and Δt the integration time step of LR run.

The rationale of the approach lies in the fact that nonlinearities of dynamics and chemistry lead to concentration fields, obtained from the HR run and averaged over the LR grid, which differ from those directly obtained from the LR run. Furthermore, the actual forcing term, HR-r, is obtained from HR by conservatively remapping the HR results onto the LR grid. It is known that, for a variety of reasons, HR-r is likely to perform better than HR when compared to data (Valari and Menut, 2008).

In the present paper the nudging technique is exclusively applied to concentration fields. The same kind of forcing can in principle be applied to the meteorological fields as well (at least velocity and temperature). However, in an online coupled model like BOLCHEM this could produce unbalances in the dynamic fields propagating into the domain that must be damped by increasing the numerical dissipation. In absence of an independent verification of the impact of these disturbances on the meteorological simulation, for the purposes of this work such forcing has been excluded. Note that forcing on the chemical species has in general a more localized effect than the forcing on meteorological fields (emission, reactions, deposition are essentially local processes). In the future, however, the forcing will be tested on the entire set of prognostic variables of the model.

3 Experimental setup

The nudging procedure is applied using the BOLCHEM model running at different horizontal resolutions over different domains.

Three different model runs were performed for the year 2005: (i) the LR ($0.5^\circ \times 0.5^\circ$, $\Delta t = 400$ s) run over Europe (6° W–44° E, 30° N–57° N), driven by boundary conditions from ECMWF and anthropogenic emissions prepared by INERIS for the CityZen project (https://wiki.met.no/cityzen/start); (ii) the HR ($0.1^\circ \times 0.1^\circ$, integration time step: 90 s) run over the Po Valley (7.95° E–12.83° E, 44.4° N–45.98° N) driven by boundary conditions taken from LR run; and (iii) the LR-N run over the same domain and with the same resolution as the LR run applying the nudging over the Po Valley every forecast hour and to all model species at all levels.

The relaxation time τ in Eq. (1) was set to 1200 s, so that in steady conditions and for a passive tracer the LR run would converge to the HR run before the updated forcing value was used. The value of $C_{\text{HR-r}}$ is updated every hour.

4 Results

The statistics of the differences in concentration for the selected species (CO, O_3, NO_2 amd PM_{10}) are used here to analyze the results of the numerical experiments. The fields considered are relative to the ground level (the first model level above the ground), but some analysis was performed at two additional levels: about 450 m a.s.l. and 900 m a.s.l. The statistics refer to the whole one-year period and to 4 three-month (seasonal) periods.

It is expected that the main effects of this technique will occur within the forcing area, although the ultimate goal is an overall improvement of the skills of the low resolution run also outside the forcing area. Therefore the effects of the nudging technique were also studied outside the Po Valley area and the analysis of the results was performed for the Po Valley region, as well as in the three rectangular frames illustrated in Fig. 1. These 4 regions will be hereon referred to as: (i) core (the forcing region); (ii) frame 1 (region limited internally by the core bounds and externally by the box: 6.7° E–14.3° E, 43.3° N–47.0° N); (iii) frame 2 (region limited internally by the frame 1 bounds and externally by the box: 6.0° E–15.1° E, 42.8° N – 47.5° N); (iv) frame 3 (region limited internally by the frame 2 bounds and externally by the box: 5.4° E–15.8° E, 42.2° N–47.9° N).

The average difference $C_{\mathrm{LR}} - C_{\mathrm{LR-N}}$ and the corresponding standard deviation fields for the one-year period are reported in Fig. 2 for the four species. The effect of nudging is evident in the core region for all the species. Outside the core this effect is more evident for PM_{10} than for CO. Moreover the difference fields show a clear seasonal trend for NO_2 and O_3, with opposite patterns (for NO_2 the largest effect is present during autumn and winter, with a minimum during summer; a reversed trend is displayed by O_3). Figure 3 shows the seasonal variation for NO_2. The effect is larger and more spread in winter than in summer.

4.1 Taylor diagrams

To better highlight the differences between LR run and LR-N run, the HR-r run is used as reference. It should be noted that the HR run covers only the forcing area and therefore the analysis performed using the Taylor diagrams is limited to the core.

The Taylor diagram provides concise two-dimensional plots of statistical properties which show how well simulated patterns match a reference (Taylor, 2001). In this case, the comparison between low resolution simulations (with and without nudging) and the reference (HR-r run) is performed. The axes refer to the standard deviation of the LR run normalised to the standard deviation of the reference. The correlation coefficient between a given field and the reference is represented by its azimuthal position, while the root mean square difference between a run and the reference (in units of standard deviation) is proportional to their distance. Therefore each point plotted on the diagram defines how close a simulation is to the reference in terms of the above statistical properties.

Figure 4 represents the Taylor diagram resulting from the comparison between run LR and HR-r (black symbols), and run LR-N and HR-r (red symbols) for the selected species and for the lowest model level. The figure clearly shows the improvement due to the nudging in terms of the increase in correlation and decrease in the centered root mean square difference for all the considered species except for O_3. The same behaviour is found at the other analysed levels (not reported here).

It is worth noting that the improvement in the model performances is fairly small as far as O_3 is concerned (the same happens at all the investigated levels), which is a consequence of the rather slight difference between the LR and HR runs. In fact the photochemical production of O_3 occurs over a typical time longer than the horizontal mixing time in the Po Valley, yielding rather similar mean concentrations in the LR and HR runs, as shown by the relatively small differences in Fig. 2.

4.2 Scatterplots and histograms

The usefulness of the nudging technique lies in the ability to influence the simulated concentrations outside the forcing area. Since Taylor analysis cannot be performed outside the forcing area, we examined the scatter plots of LR vs. LR-N and the histograms of LR-N minus LR. Scatterplots and histograms in the forced region and in the frames outside are reported in Figs. 5 to 8. The concentration values have been normalised to C_{HR} in the forcing area for the periods of interest (one year, three months).

In this way we clearly observe the scattering of the concentration values in the LR-N run with respect to the LR run for different species and in the different analysis areas. The first feature to be noted is that the level of scattering differs greately from one species to another. In particular is more marked for NO_2 than for O_3. In addition for all species the scatter decreases with increasing distance from the core, becoming significant only for smaller concentration values in outer regions.

At the same time the histograms show that the difference distribution is far from being Gaussian, with the appearance of long tails. The occurrence of large differences is greater than for a Gaussian process. In fact, the computed kurtosis (see Table 1) shows large departures from the Gaussian value of 3, which also increases with the distance from the core. This means that the forcing can occasionally have a strong influence outside the forcing region.

The different species also show different seasonal behaviours. Seasonal scatterplots show that the most relevant seasonality is present in the case of NO_2, reported in Fig. 9, with a standard deviation of 0.26 during summer and 0.36 during winter, the occurrence of large fluctuations being more likely in winter. Of the species, the least significant dependence on the season has been found for PM_{10} (not shown).

A synthetic representation of the effects of nudging outside the forcing area is shown in Fig. 10, where the standard deviation of the differences, normalised to the average concentration in the forcing area is reported as function of the frame number. Differences among the species can be recognised, but the overall behaviour is similar, clearly highlighting the spread of the effect of forcing.

For all the species, the differences are larger in the forced region and decrease with increasing distance. Quantitatively, in frame 3 the differences are still about 0.05 of the mean concentration in the inner area, corresponding to a decrease of about 20% of the effect in the core area.

5 Conclusions

A new method for allowing different models with different spatial resolutions to interact has been investigated. A numerical experiment has been performed, using two runs of BOLCHEM at different spatial resolutions focusing on the Po Valley hot-spot.

The application of the nudging technique to force the low resolution model towards the high resolution run has thrown light on the following:

- the performance of the nudged coarse model is significantly closer to that of the fine resolution model;
- the propagation of the effect of forcing covers a wide area outside the forcing region;
- seasonal effects on propagation are identified for some species, but not for all of them: in general as processes of transformation become more relevant (local chemistry/deposition dominates), the propagation is weaker (as for ozone in summer); for slowly reacting/non-reacting species (as for particles, or NO_2 in winter) advection is important, affecting more the differences outside the forcing region (for instance, preferred transport towards the Adriatic Sea and the northern Tyrrhenian basin is evident in the NO_2 standard deviation map for winter, see Fig. 3).

In this work the values of the parameters Δt and τ were fixed as stated in Sect. 3. Different choices of the parameters can be exploited in order to obtain the best agreement with the reference (which should be either a model or observations).

The point to be stressed again is that this technique can be applied not only to the same model running at different resolutions, but, more importantly, to two different models (e.g. a global, coarse resolution model and a regional, high resolution model).

Using two models with different chemical mechanisms requires considerable care, for instance, in matching chemical mechanisms and the selection of key species for the forcing. The type and number of species necessary should be further investigated. Moreover, the different representation of the vertical structure of the boundary layer must be accounted for.

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Table 1. Kurtosis of the concentration difference between LR and LR-N runs calculated for the year ensemble for each species and for each frame.

	O_3	PM_{10}	CO	NO_2
core	10.9874	4.93241	2.91300	5.37418
frame 1	22.1872	14.7003	49.8091	32.5261
frame 2	49.7680	23.8663	42.8987	82.9959
frame 3	191.047	33.1673	71.7127	132.741

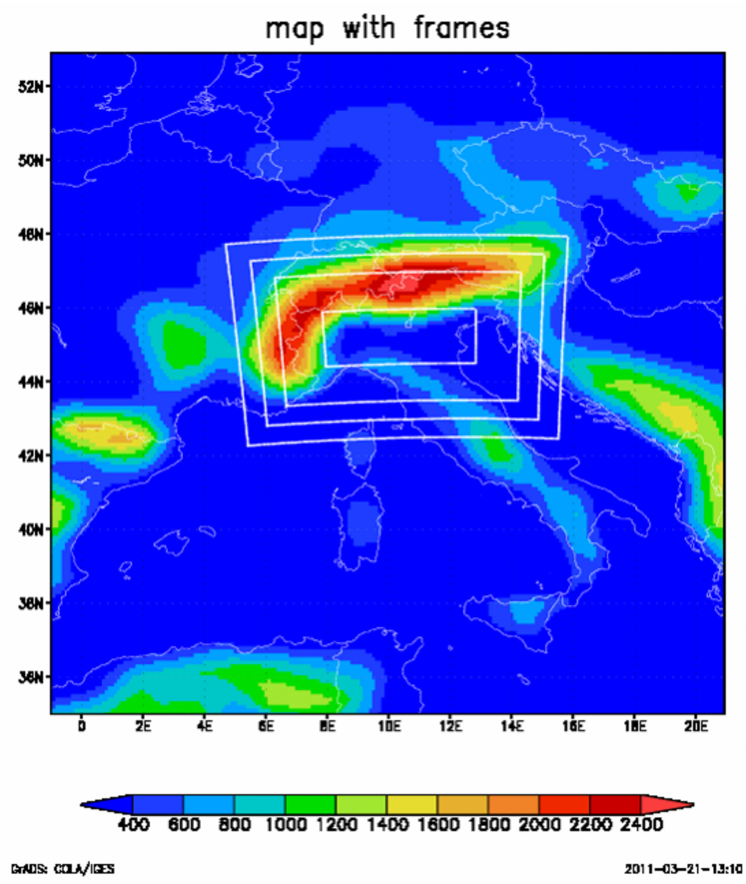

Fig. 1. Po Valley orography map showing surface elevation in meters. The white boxes represent: the forcing area (inner box) and the 3 progressively larger frames on which the analysis was performed.

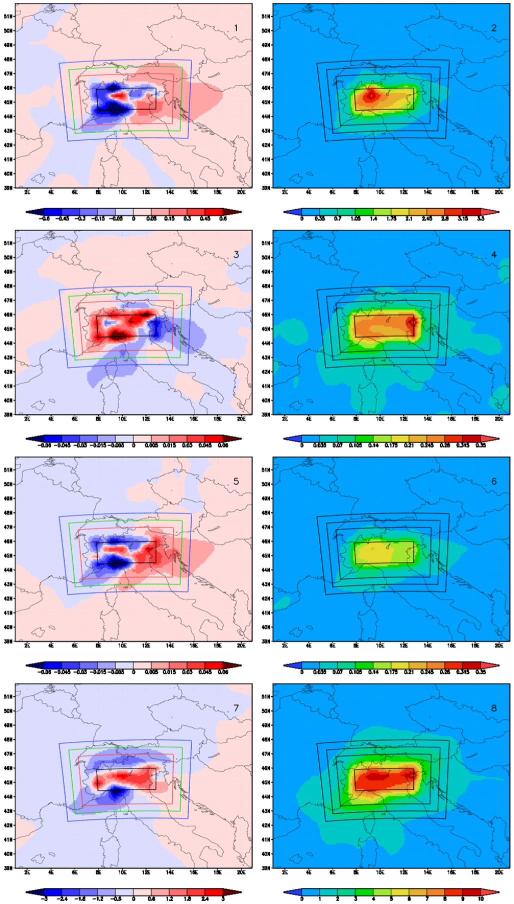

Fig. 2. Yearly average and standard deviation of concentration difference (LR-N minus LR) for the four species studied. Panels refer to: CO (1–2), O_3 (3–4), NO_2 (5–6) and PM_{10} (7–8).

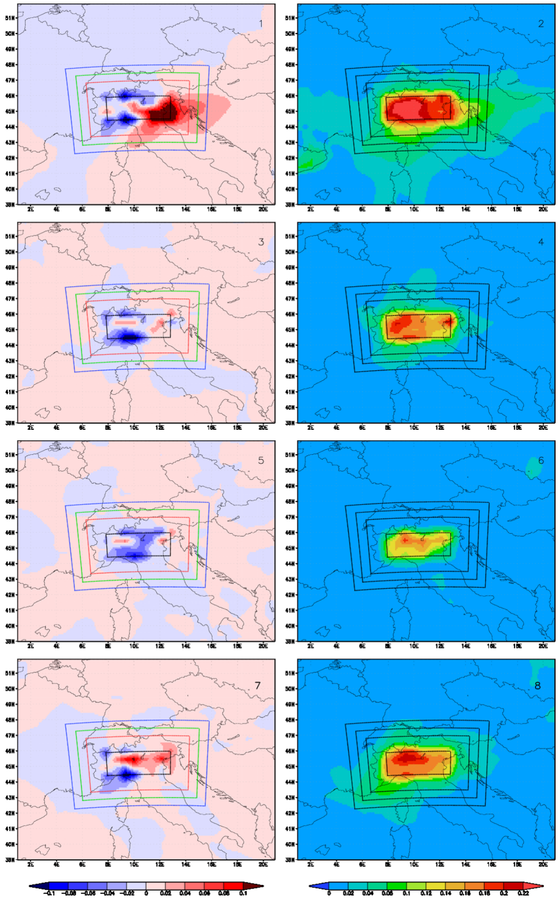

Fig. 3. Seasonal average and standard deviation of concentration difference (LR-N minus LR) for NO_2. Panels refer to: winter (1–2), spring (3–4), summer (5–6) and autumn (7–8).

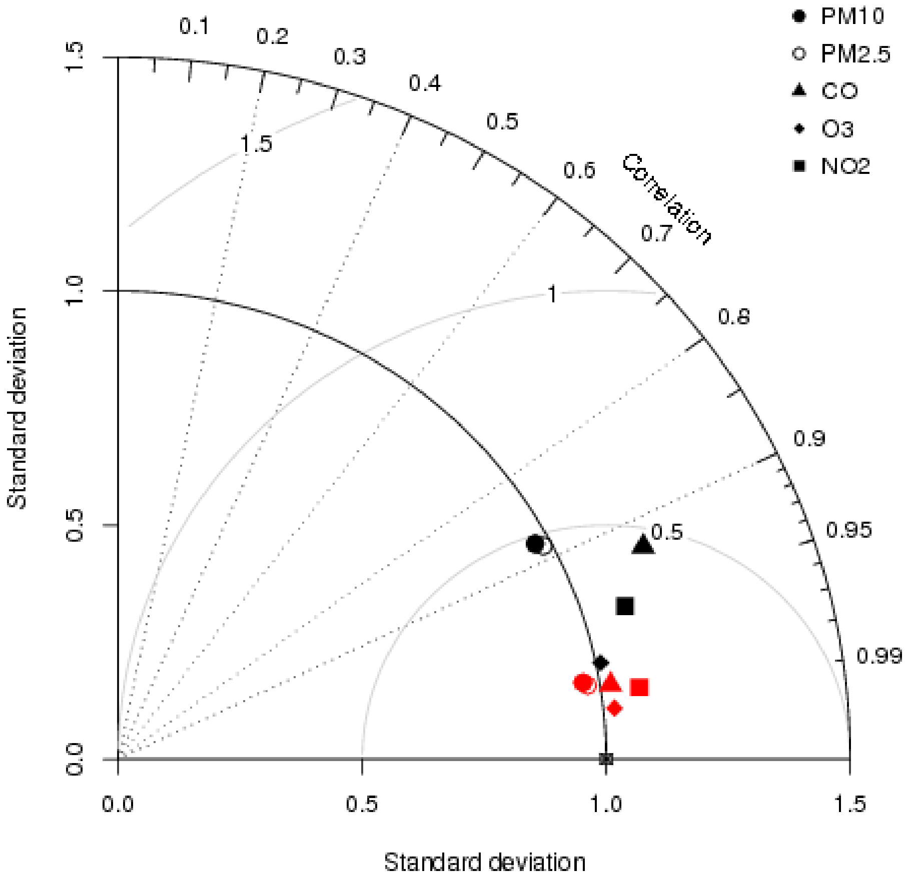

Fig. 4. Taylor diagram showing the performance of the LR-N simulations (red symbols) with respect to the HR-r (reference). Black symbols refer to the LR simulations.

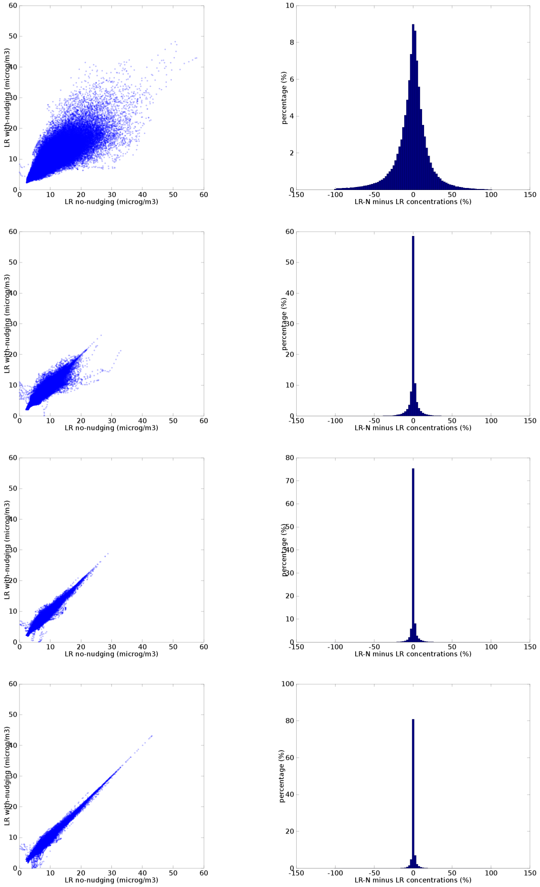

Fig. 5. LR-N vs. LR scatter plot (left panels) and the corresponding histogram (right panels) of the concentration differences for CO. From top to bottom: core region, frames 1 to 3.

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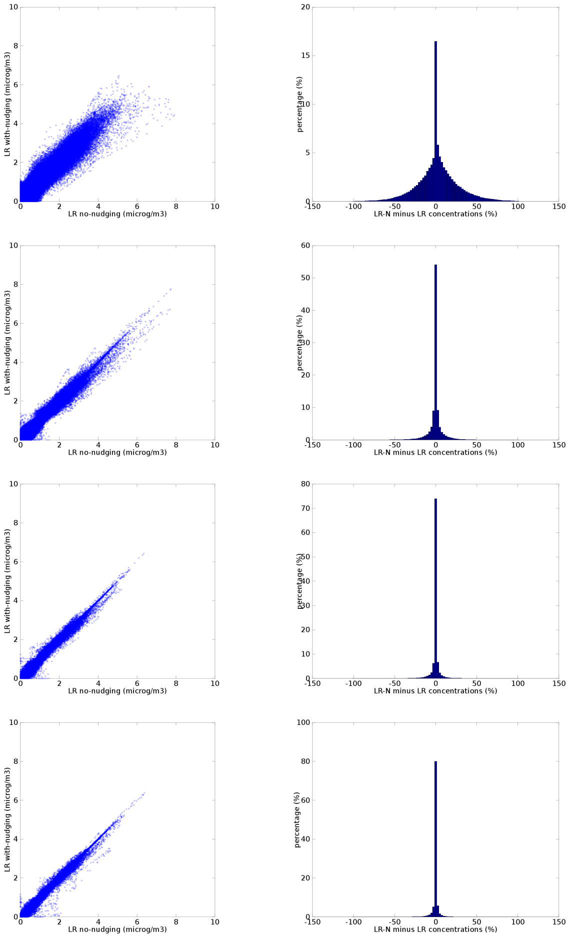

Fig. 6. As in Fig. 5, but for O_3.

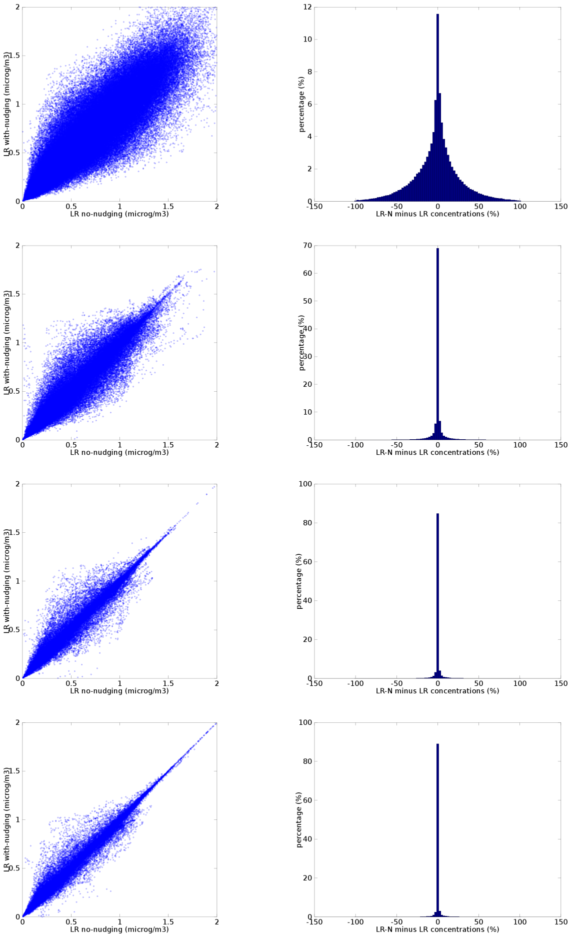

Fig. 7. As in Fig. 5, but for NO_2.

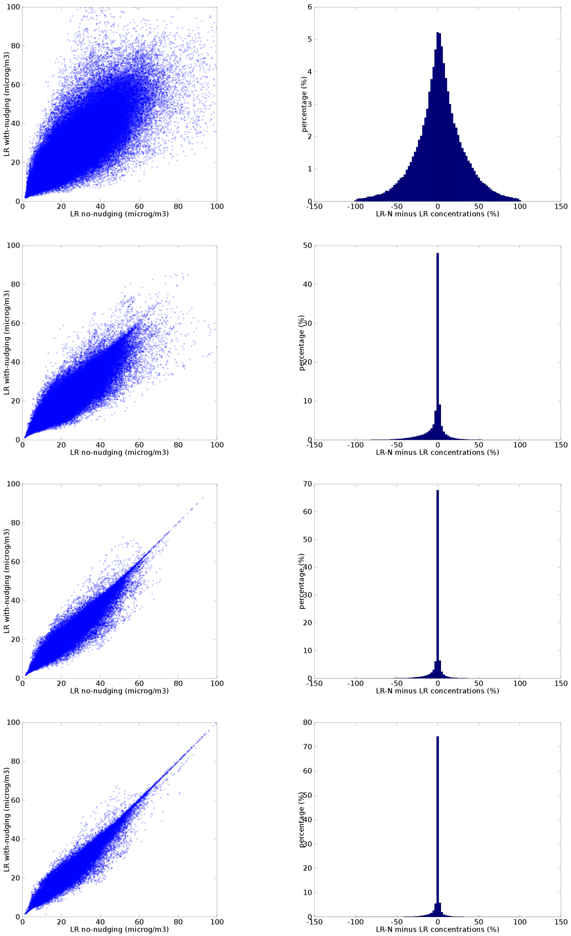

Fig. 8. As in Fig. 5, but for PM_{10}.

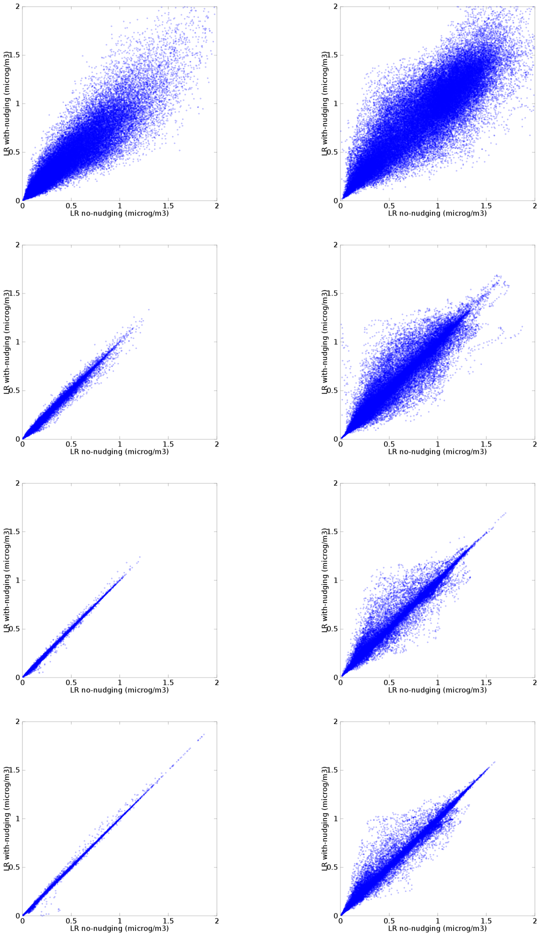

Fig. 9. Seasonal scatterplots relative to NO_2 for summer (left panels) and winter (right panels).

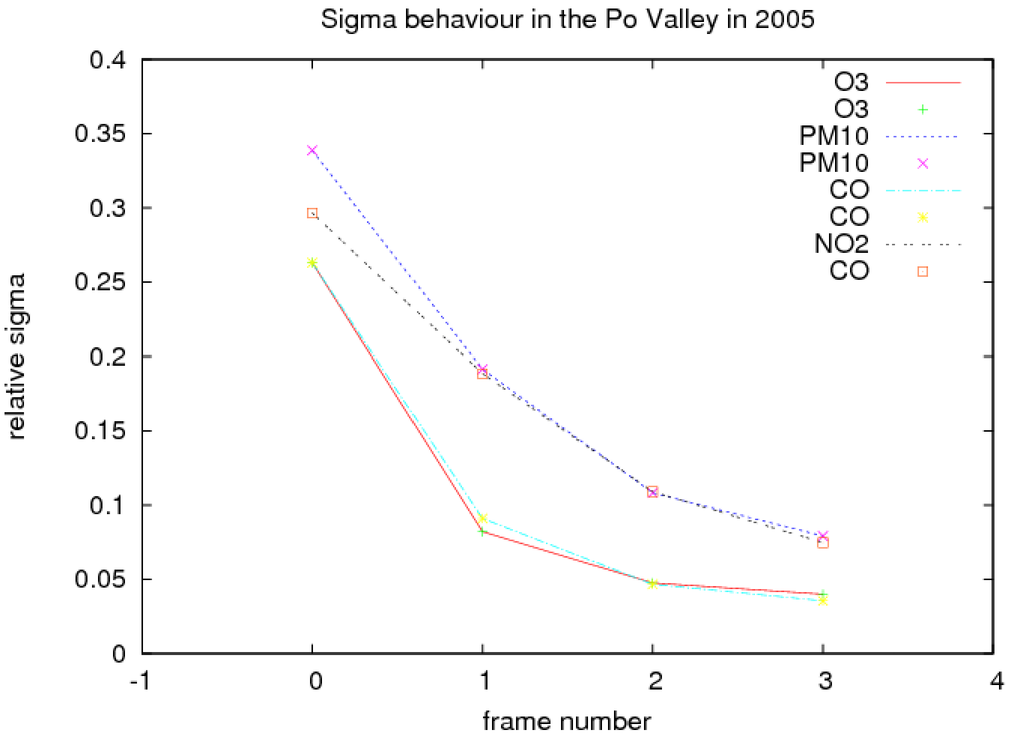

Fig. 10. Variation of the normalised standard deviation with the distance from the core. The numbers in abscissa correspond to the core (0), the frame 1 (1), the frame 2 (2) and the frame 3 (3).