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COMPUTATIONAL TESTS TO IMPROVE THE SPATIAL RESOLUTION OF THE ATMOSPHERIC TRANSFER MATRICES IN THE INTEGRATED ASSESSMENT MODEL MINNI

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Abstract: This paper presents the update of the atmospheric transfer matrices in the MINNI integrated assessment modelling system for air quality in Italy. The performed tests demonstrated the feasibility of improving the horizontal resolution from 20 km to 4 km on the ENEA CRESCO HPC infrastructure. This allows reaching the spatial detail of state-of-art operational chemical-transport modelling systems in Europe but offering a faster way to estimate the efficacy of different air pollution control policies in reducing the impact on human health and the environment.

Key words: *atmospheric transfer matrices, integrated assessment model, high performance computing, source-receptor relationships*

INTRODUCTION

Air pollution control policies aim to improve air quality to mitigate anthropogenic emissions' negative impacts on human health and the environment. Chemical-transport air quality models represent valuable tools to evaluate concentrations/depositions of air pollutants derived from anthropogenic activities. These models are getting more and more sophisticated, requiring both specialist skills and a considerable amount of computational time, while air quality policymakers often require quick responses and simple messages about the impacts of different policy scenarios. Hence, there is an urgent need for computationally efficient tools, providing an integrated assessment of the different types of impact (both the environment and health) of the various policies to improve air quality (Milando et al., 2016). Reduced form models, providing simplified relationships between emissions and concentrations/depositions/related impacts, have been used for the purpose (Arndt and Carmichael, 1995; Seibert and Frank, 2004; Foley et al., 2014).

A possible scheme for simplifying the chemical transport and diffusion dynamics is the ATMs (Atmospheric Transfer Matrices) approach, implemented in GAINS (Amann et al., 2011) and derived from the EMEP source-receptor relationships (Bartnicki, 1999). Within the MINNI project (Mircea et al., 2014; Vitali et al., 2019), ENEA has developed an integrated assessment tool, the GAINS-Italy model (D'Elia et al., 2009; 2018; Ciucci et al., 2016), where ATMs (Briganti et al., 2011) allow fast responses in terms of impact to different policy emission scenarios. Based on multiple simulations of the complete form of the chemical-transport model, the ATMs calculation requires significant resources and execution times. The present work aims to discuss the sensitivity tests we conducted on different values of a temporal step of integration (DTS, from 30 s to 200 s), spatial resolution (8 km and 4 km) and paradigm option for parallelization of the ENEA CRESCO HPC Infrastructure (Iannone et al., 2019), aimed to minimize the calculation time.

METHODOLOGY

ATMs are source/receptor relationships, linking the emissions of a specific pollutant in a given geographical area (source) to the relative concentrations/depositions and impacts calculated at a given point (receptor), simplifying the atmospheric processes involved (meteorological dynamics, physical and chemical processes on pollutants). In the case of GAINS-Italy, the source terms are the aggregate emissions on each of the 20 Italian administrative regions, while the receptors coincide with the model calculation grid's points.

The ATMs describe the response of the concentrations/depositions at a given grid point/receptor to the

variation of the emissions of each region/source, obtained by applying a perturbation to the emissions of each of the primary compounds of interest, namely SO_X, NO_X, NH_3, NMVOC and PM_{10}, and were calculated for 8 pollution indicators (sulphur deposition (TS), total nitrogen deposition (TN), reduced nitrogen deposition (TNH), concentrations of $PM_{2.5}$, PM_{10}, NO_2, O_3 as SOMO35 (the sum of the daily maxima of 8-hour running average over 35 ppb) and as AOT40 (the accumulated amount of ozone over the threshold value of 40 ppb)). A complete simulation of the Atmospheric Modelling System (AMS) of the MINNI model has been conducted for each emitted compound.
ATMs are a sort of Taylor expansion of function with 100 indipendent variables (the emissions of pollutant "p" in the "r" region, Epr). The first order approximation requires the perturbation of each single variable. The second order describes the perturbations of two independent variable at the same time. We considered first- and second-order relationships to be an acceptable reduced form of the complete model.
The calculation of ATMs requires significant resources and execution times on the ENEA CRESCO HPC Infrastructure. To minimize the calculation time, sensitivity tests were conducted on different values of temporal step of integration (DTS, from 30 s to 200 s), spatial resolution (8 km and 4 km) and paradigm option for parallelization, using a reference emission scenario (BS) and a perturbed emission scenario (AS) on three Regions with high emissions (Lombardia, Lazio and Campania). The model setup used to perform all the tests is summarized in Table 1.

Table 1. Setup of the model.

	Description	
Parameters	**4 km horiz. res.**	**8 km horiz. res.**
Reference Emission Scenario (BS)	ISPRA 2015 national inventory, Emission Manager (EMGR) v. 6.7	
Altered Emission Scenario (AS)	- 25% emissions over Lombardia-Lazio-Campania	
Meteorology	MINNI scenario 2015	Interpolated from 4km
Version of chemical-transport model (FARM)	4.14	
Parallelization paradigm	pure MPI, hybrid MPI/OMP with 4 OMP dedicated cores, hybrid MPI/OMP with 8 OMP dedicated cores	
Cresco section	Cresco6	
DTS	30, 60, 100, 200, 300 s	
Considered species	O_3, NO_2, PM2.5, PM10, TS, TN, TNH at ground-level	
Postprocessing	Annual averages	

RESULTS

We considered different DTS where the value of 30 s may be viewed as the best choice to guarantee maximum accuracy, up to 4 km horizontal resolution. Table 2 shows the maximum errors obtained on annually-averaged fields from the base scenario (BS), varying DTS from 60 s to 200 s. The absolute differences are evaluated by subtracting mean values produced with DTS=30 s

$$\mathrm{diff}=\max\{\ |\ \langle \mathrm{field}(x,y)\rangle_{DTS} - \langle \mathrm{field}(x,y)\rangle_{DTS=30s}\ |\ \big|\ (x,y)\in D\} \quad (1)$$

where, the maximum of the absolute values is calculated over the whole grid domain, D. Negative values in the table mean underestimation induced by non-optimal DTS.
Table 3 shows the maximum errors on the difference between altered case (AS) and BS, in the function of DTS, that is:

$$\mathrm{diff}(DTS)=\max\{\ |\ \langle \mathrm{field}(x,y)\rangle_{AS,DTS} - \langle \mathrm{field}(x,y)\rangle_{BS,DTS}\ |\ \big|\ (x,y)\in D\ \} \quad (2)$$

Table 2. BS, annual averages, minimum and maximum values and maximum errors for each species on the domains at 8 and 4 km of resolution (differences DTSXXX-DTS030).

				8KM			
SPEC	**UNIT**	**MIN**	**MAX**	**DTS060**	**DTS100**	**DTS200**	**DTS300**
O_3	μg/m^3	38.294	94.568	-1.029	-2.356	-5.55	-8.351
NO_2	μg/m^3	0.303	49.082	0.284	0.592	1.147	1.56
PM25	μg/m^3	2.488	29.078	-0.097	-0.224	-0.533	-0.818
PM10	μg/m^3	3.249	30.392	-0.105	-0.242	-0.575	-0.88
TS	mg/m^2/h	0.0094	4.3085	0.0915	0.216	0.5458	0.9171
TN	mg/m^2/h	0.0059	0.0845	-0.0003	-0.0008	-0.0021	-0.0033
TNH	mg/m^2/h	0.0004	0.5867	0.0005	0.0011	0.0027	0.0041

				4KM		
SPEC	**UNIT**	**MIN**	**MAX**	**DTS060**	**DTS100**	**DTS200**
O_3	μg/m^3	25.598	97.85	1.493	3.423	7.256
NO_2	μg/m^3	0.451	67.708	0.889	1.931	4.124
PM25	μg/m^3	2.636	41.994	0.239	0.561	1.388
PM10	μg/m^3	3.487	44.632	0.236	0.553	1.379
TS	mg/m^2/h	0.0114	14.129	0.5213	1.2523	3.4059
TN	mg/m^2/h	0.0077	0.1018	0.0008	0.0018	0.004
TNH	mg/m^2/h	0.0003	0.6109	0.0015	0.0034	0.0076

Table 3. Differences AS-BS, annual averages, minimum, maximum values and maximum errors for each species on the domains at 8 and 4 km of resolution, in function of DTS.

				8KM			
SPEC	**UNIT**	**MIN**	**MAX**	**DTS060**	**DTS100**	**DTS200**	**DTS300**
O_3	μg/m^3	-0.1684	4.6066	-0.02315	-0.0536	-0.12835	-0.18596
NO_2	μg/m^3	-7.6263	0.0159	0.02864	0.06611	0.15899	0.23071
PM25	μg/m^3	-0.478	0.00067	0.00511	0.01175	0.02701	0.04004
PM10	μg/m^3	-0.478	0.00073	0.00508	0.01173	0.02699	0.04001
TS	mg/m^2/h	-0.00003	0.00002	0.00003	-0.00019	-0.00003	-0.00036
TN	mg/m^2/h	-0.00926	0	0.00006	0.00013	0.00034	0.00053
TNH	mg/m^2/h	-0.00025	0.00138	-0.00003	-0.00003	-0.00007	-0.00009

				4KM		
SPEC	**UNIT**	**MIN**	**MAX**	**DTS060**	**DTS100**	**DTS200**
O_3	μg/m^3	-0.1786	5.0665	0.03806	0.08656	0.16426
NO_2	μg/m^3	-8.7737	0.02916	0.04562	0.10589	0.20668
PM25	μg/m^3	-0.48553	0.0102	0.00749	0.01702	0.0362
PM10	μg/m^3	-0.48554	0.01025	0.0075	0.017	0.03623
TS	mg/m^2/h	-0.00007	0.00002	0.00011	0.00007	0.00048
TN	mg/m^2/h	-0.00987	0	0.00007	0.00018	0.00042
TNH	mg/m^2/h	-0.00038	0.0015	0.00002	0.00004	0,00007

As previously underlined, the maximum absolute values are computed over the domain, and the negative sign means underestimation.

As regards the calculation speed, Fig. 1 illustrates the speeds for three paradigm options: pure MPI, hybrid MPI/OMP with 4 OMP dedicated cores, and hybrid MPI/OMP with 8 OMP dedicated cores.

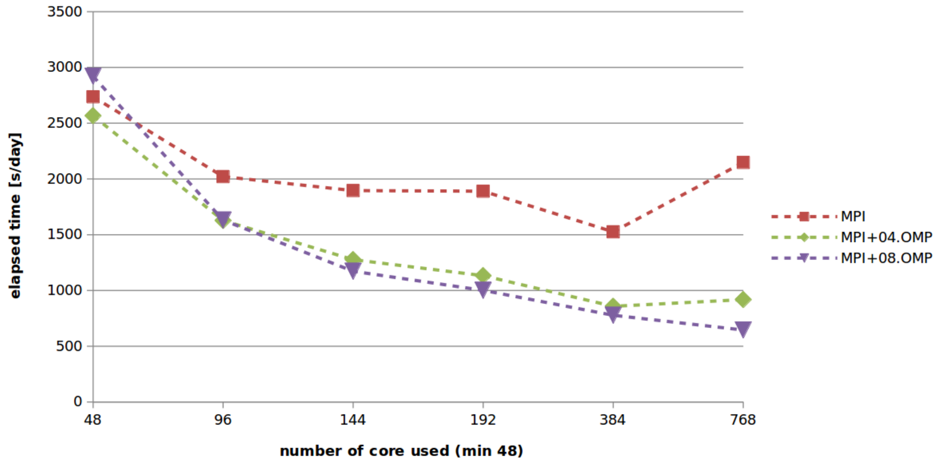

Figure 1. Calculation speed (elapsed time) in seconds per day for the simulation with a horizontal spatial resolution of 4x4 km.

A multiple of 48 core was chosen to occupy the nodes entirely. The aim is to guarantee to complete each simulation in 24 hours: being each annual run splitted in 12 parallel runs, it is enough to get an elapsed time of 2750 s/day. For this purpose, the most efficient configuration, guaranteeing to end each simulation in 24 hours, uses 48 core with 4 OMP dedicated ones. Pure MPI does not seem much efficient, not being FARM a complete vector code.

CONCLUSIONS

In this work, to minimize the significant calculation time required by ATMs, several sensitivity tests were conducted to explore different DTS values, spatial resolutions and paradigm options for parallelization.
Increasing the DTS leads to lower calculation time but higher errors on absolute concentrations/depositions, suggesting adopting a small value (60 s) for the DTS in the BS's complete simulation. The DTS and spatial resolution produce lower errors in concentration/deposition differences between AS and BS than on BS concentrations, suggesting that a DTS of 150 s is sustainable for the emission abatement runs (ASs). It is worth noting that the possibility to increase DTS allows to improve the horizontal resolution to 4 km with a sustainable computational effort in CRESCO and thus reaching the spatial detail of the complete AMS–MINNI, which is the state-of-art level of operational chemical-transport modelling systems in Europe.

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