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

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ABSTRACT

This poster 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.

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THE ATMOSPHERIC TRANSFER MATRICES (ATMs) FRAMEWORK

ATMs are simplified models implemented in GAINS (Amann et al., 2011) and specifically designed to giving to air quality policymakers quick responses and simple messages about the impacts of different policy scenarios. Within the MINNI project, ENEA has developed an integrated assessment tool, the GAINS-Italy model (D'Elia et al., 2009) based on ATMs (Briganti et al., 2011).

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 of SO_X, NO_X, NH_3, NMVOC and PM10 on each of the 20 Italian administrative regions, while the receptors coincide with the model calculation grid points. ATMs are a sort of Taylor expansion of function with 100 independent variables (20 regions x 5 precursors). 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: second order coefficient are supposed mainly local, in order to significantly reduce the elapsed time and preserve the necessary accuracy.

	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	

Table 1 – Model setup.

The ATM calculation requires significant resources and execution times on the ENEA CRESCO HPC Infrastructure (Iannone et al., 2019). To minimize the calculation time, sensitivity tests were conducted on different values of temporal integration step (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. Based on multiple simulations of the complete form of the chemical-transport model, the ATM 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, spatial resolution and paradigm option for parallelization of the ENEA CRESCO HPC Infrastructure, aimed to minimize the calculation time.

RESULTS

The aim is to determine the best configuration to obtain ATMs at the lowest possible resolution, close to or equal to MINNI full run.

Concentration accuracy.

We firstly determined the impact of DTS on concentration accuracy.

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

$$diff = max\{|C_{DTS}(x,y) - C_{30s}(x,y)|\}$$

where, the maximum of the absolute values is calculated over the whole grid domain. Negative values in the table mean underestimation induced by non-optimal DTS.

		8 km					
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
		4 km					
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 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).

Impact of DTS value on concentration differences.

To compute ATMs with enough accuracy, we also need an estimation of the impact of the errors induced by DTS on the differences between altered case (AS) and BS.

$$diff(DTS) = max\{|C^{AS}_{DTS}(x,y) - C^{BS}_{DTS}(x,y)|\}$$

Table 3 shows the maximum errors on the differences AS-BS, as function of DTS.

As previously underlined, the maximum absolute values are computed over the domain, and the negative sign means underestimation. It is clear as the DTS impact on differences AS-BS is very small, in comparison with values in Table 2. That is a crucial conclusion: we can accept coarser DTS and still preserve enough accuracy.

		8 km					
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
		4 km					
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	

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.

Scaling and calculation speed.

Fig. 1 illustrates the speeds for three paradigm options used in this work: pure MPI, hybrid MPI/OMP with 4 OMP dedicated cores, and hybrid MPI/OMP with 8 OMP dedicated cores. A multiple of 48 core was chosen to occupy the nodes entirely. Tests are performed with Intel/Intel17 default module. 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 4.14 a full vector code.

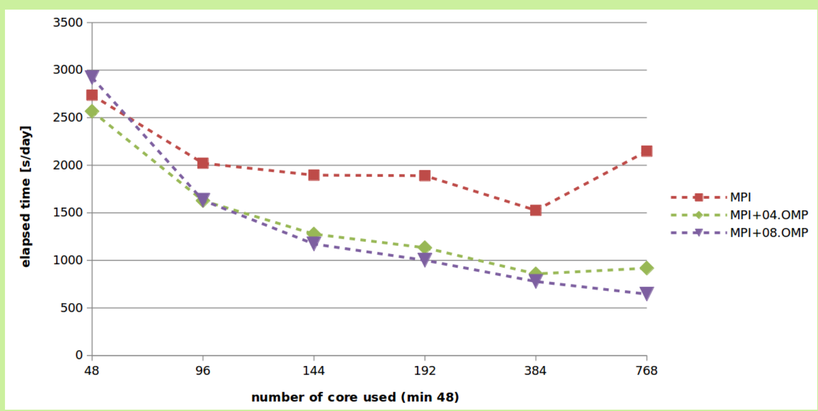

Figure 1- Calculation speed (elapsed time) in seconds per day for the simulation with a horizontal spatial resolution of 4x4 km.

CRESCO6 architecture.

The Portici CRESCO6 cluster is a computing system made up of 434 nodes. Each node has: i) two 24-core sockets with Intel (R) Xeon (R) Platinum 8160 processor with 2.10 GHz clock frequency and 192 GB of RAM; ii) An Intel Omni-Path 100 Gbs^{-1} interface; iii) Two GbE interfaces; iv) BMC/IPMI 1.8 support and remote console management software. We therefore have 20832 cores connected to each other by a broadband and low latency network based on Intel Omni-Path at 100 Gbs^{-1}.

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.

References

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