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Technical Assistance for Improving Air Quality and Raising Public Awareness in Cities in Turkey - CITYAIR (in line with CAFE Directive)

Contract N° TR2017 ESOP MI A3 01/SER/01

Report on

Activity 2.3.b – Suggestions for the Improvements of the Technical Capabilities of MoEU Regarding the Connection Between the National/Local Inventories and the Models

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	Activity 2.3.b – Suggestions for the Improvements of the Technical Capabilities of MoEU Regarding the Connection Between the National/Local Inventories and the Models
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1. Computational Ability for Atmospheric Modeling

Air quality models mathematically solve all chemical and physical processes in the atmosphere to calculate the following processes.

- Emissions released to the Atmosphere
- Chemical reactions of the emissions in the atmosphere
- Physical transport of emissions in the horizontal and vertical plane
- Calculates dry and wet collapse process of the emissions.

This modelling system consists of the emission model, meteorology model and air quality model. To solve the resulting partial differential equations, the initial and boundary conditions must be known. For instance, a modelling study for Istanbul needs to run the following models.

- Meteorological model: European Model Area 36 x 36 km, Turkey Model Area 12 x 12 km, İstanbul Model Area 4x4 km
 - 36x36 km: 100x180x34 (Row x colon x layer numbers) = 612.000 cell
 - 12x12 km: 79x160x34 (Row x colon x layer numbers) = 429.760 cell
 - 4x4 km: 85x127x34 (Row x colon x layer numbers) = 367.030 cell

When the average 100 parameters are solved and the time step is assumed to be 10 at the simulated hour (most of the time step reaches 2min), the total number of accounts is¹:

- 36x36 km: 612.000.000 count / hour
- 12x12 km: 429.760.000 count / hour
- 4x4 km: 367.030.000 count / hour

When the study is a 12-month simulation (8760 hours), the calculation required for the meteorological model calculates a total of 12,341 Trillion.

- 36x36 km: 5.361.120.000.000 count
- 12x12 km: 3.764.697.600.000 count
- 4x4 km: 3.215.182.800.000 count
- The air quality model has the same configuration with the WRF. When the average 200 parameters are solved and the time step is assumed to be 10 per simulated hour (mostly time step reaches 2min), the total number of accounts is 24,682 Trillion.

¹ For a single account, the number of accounts varies with the calculated parameter



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- 36x36 km: 10.722.240.000.000 count
- 12x12 km: 7.529.395.200.000 count
- 4x4 km: 6.430.365.600.000 count

As a result, a total calculation exceeding 36 Trillion is required for a 1-year simulation. A CMAQ study for a province requires at least 3 scenario simulations. In other words, the necessity of a calculation exceeding 120 trillion in total arises. When a similar study is needed for more than one province at the same time, this count reaches to finds quadrillions. The calculation time of such a study on the computer depends on many parameters. Below, a 1 month CMAQ simulation runs in 36 hours on a Linux machine which has a 48 core 96 gb ram and a 5TB hard drive. WRF, Dumani MCIP and CMAQ work in total 700 hours.

An example of the system to be purchased may be the Cheyenne machine at the National Center for Atmospheric Research (NCAR). https://akirakyle.com/WRF_benchmarks/results.html

Related video is: https://youtu.be/ycNQ_wqsWFc

A machine running WRF must have a total of 145,152 cores and 313 Tb of memory.

Cheyenne
<ul style="list-style-type: none">● 4,032 computation nodes<ul style="list-style-type: none">○ Dual-socket nodes, 18 cores per socket<ul style="list-style-type: none">■ 145,152 total processor cores○ 2.3-GHz Intel Xeon E5-2697V4 (Broadwell) processors<ul style="list-style-type: none">■ 16 flops per clock○ 5.34 peak petaflops● 313 TB total system memory<ul style="list-style-type: none">○ 64 GB/node on 3,168 nodes, DDR4-2400○ 128 GB/node on 864 nodes, DDR4-2400● Mellanox EDR InfiniBand high-speed interconnect<ul style="list-style-type: none">○ Partial 9D Enhanced Hypercube single-plane interconnect topology○ Bandwidth: 25 GBps bidirectional per link○ Latency: MPI ping-pong < 1 μs; hardware link 130 ns

Table 1: Features of Cheyenne machine at the National Center for Atmospheric Research (NCAR)



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Performance tests on this machine are also presented below.

case	e _{We}	e _{sn}	total gridpoints	timestep	run hours
conus12km	425	300	127,500	72	3
conus2.5km	1901	1301	2,473,201	15	6
new_conus12km	425	300	127,500	72	6
new_conus2.5km	1901	1301	2,473,201	15	6
maria1km	3665	2894	10,606,510	3	1
maria3km	1396	1384	1,932,064	9	3

Table 2: Performance of Cheyenne machine at the National Center for Atmospheric Research (NCAR)

Maria 1 km test simulation results are presented below.

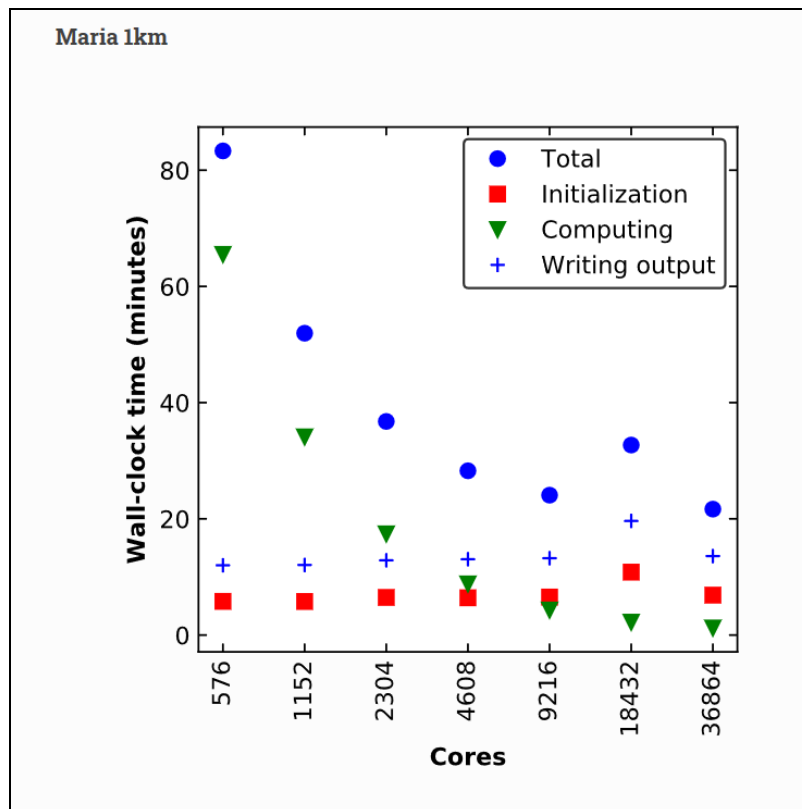


Table 3: Maria 1 km test simulation results



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According to this graph, the 576 core machine simulates approximately 65 minutes, while a 1152 core machine performs in 38 minutes and a 2304 core machine performs in 20 minutes.² After 2304 cores, the gain rate decreases.

It is recommended that the machine to be used has a minimum of 2300 cores and a minimum of 8gb of memory per core. The hard disk requirement can also be calculated by considering the simulations.

In order to run the forecast according to the state of the art's methodology in the air quality modelling community, a Linux high performance computing cluster with the following requirement is highly recommended:

- a large range of libraries in order to run the dedicated scripts and tools associated to the model
- a 24/7 supervision of the cluster,
- a backup system in order to avoid the loss of essential data.
- A system of archives of previous forecast outputs
- Robustness and reliability of the cluster.
- About 200 cpu regarding the set-up proposed for the air quality forecast production over Turkey.

Significant storage is necessary (Several Tb) with a possibility to upgrade this volume according to the policy of retention of the production and the archive system.

In addition, the IT environment should be as follow:

1) intel/17.1.132

2) intelmpi/5.1.2.150

3) phdf5/1.8.18

4) netcdf/4.4.1

5) cdo/1.7.2

6) nco/4.6.2

² 1 hour simulation



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- 7) pnetcdf/1.7.0
- 8) grib_api/1.18.0
- 9) xz/5.2.2
- 10) zlib/1.2.8
- 11) szip/2.1
- 12) bzip2/1.0.6
- 13) armadillo/7.500.0
- 14) gdal/2.1.1
- 15) geos/3.6.0
- 16) gmt/5.3.1
- 17) pcre/8.39
- 18) curl/7.51.0
- 19) libxml2/2.9.4
- 20) proj/4.9.3
- 21) R/3.3.2
- 22) blitz/0.10
- 23) python/2.7.5



2. French Air Quality Forecast Processes as an Example for the Future Modelling Works

This report should be seen in the context of the description of the modelling tools that appeared in the previous report on activity 2.3a. It provides clarification in terms of IT requirements and organization of the simulations for scenario modelling using the WRF/CMAQ chain as well as forecast modelling using IFS/CHIMERE models. On behalf of France expertise based on the current framework of French national air quality modelling and forecasting, additional comments are given hereafter as an example:

In order to run an operational forecast system, several processes must be set and launch automatically for both national or local scale:

- i) Compilation of emission data for the period of simulation.

The French operation forecast system (https://www.prevoir.org/en/general_prev.php) download once a year **from CAMS- (Copernicus Atmosphere Monitoring Service)** the **regional yearly** gridded emission dataset for the **anthropic** emission (10km long*5 km lat) on a selected area.

Concerning the temporal profile, the air quality model provides a country database of temporal profiles (that must be completed for Turkey) for the different anthropic emission sectors. Once completed, this database may be upgraded if needed once a year in order to consider recent changes.

The process is then launched daily to compute the anthropic emission for the 3 days forecast period:

- Compute_anthropicemission_process.

Then, the needed following processes are also launched daily and give an emission value for each pollutant for each grid cell at an hourly resolution.

- Compute_biogenicemission_process (totally computed from the model with no connection to another database)
- Compute_seasaltemission_process (totally computed from the model with no connection to another database)
- Compute_fireemission_process (computed from the model with connection to the daily CAMS fire emission database in relation with satellite observations)
- Compute_dustemission_process (totally computed from the model with no connection to another database)

Regarding Turkey national air quality forecast, the only adaptation of this system is to have access to the accurate yearly and spatialised anthropic emission (from Turkish national inventory regarding national AQ forecast and/or from local inventory regarding target city AQ forecast) and complete the country temporal emission profile of the model for Turkey.



ii) Compilation of Meteorological data from IFS/ECMWF

The needed following processes are launched daily:

- Get_IFS_data_process (get and store IFS data). This involves setting up a data flow between ECMWF and the AQ forecast server.
- Preprocessing_meteo_process: projection, model grid interpolation from the IFS data.

iii) Boundary Condition: 40km ->10km->4km résolution : From Global to Regional and/or local scale forecast.

The needed following processes are launched daily:

- analyse.sh_For_each_pollutant : provide the initial pollutant fields in all the domains using a combination of observed and modelled data.
- boundary_condition_process : transfert data on borders from mother domain to child domain.

iv) Daily Model Computation on AQ forecast server.

v) Daily Model statistical adaptation.

This process applies a correction on the raw output forecast using statistical learning of model errors at each grid point.

i) Daily map postprocessing.

This process makes it possible to develop air quality maps for different indicators and transfer them automatically to a dedicated website.



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