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The “Demokritos” web-based air quality forecasting system for the Greater Athens Area

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Abstract:
The present paper describes the operational air quality forecasting web-based system currently under development by the Environmental Research Laboratory of NCSR “Demokritos”. The system integrates three major computational modules and it is configured to apply on the Greater Athens Area, producing meteorological and air quality predictions on a high spatial resolution (1 x 1 km$^2$) and for a 72-hours time horizon with 1-hour time step in advance. A case study, as an example of the forecasting ability of the developed system, is provided for February 17 and April 8, 2008. The first date was chosen as it was an extremely cold day for the area with extensive snowfall and varying emission sources. The second date was selected randomly as a business as usual scenario.

Keywords: meteorology, air quality, high resolution forecasting web-based system.

1. INTRODUCTION

Environmental informatics presently is merely the way to link meteorology and pollution sources with personal exposure and determine the impact on human health. More importantly, it is a decision aiding tool for local authorities to predict potential atmospheric pollution problems, optimize actions and policy making activities so as to produce the maximum health benefit. Under current legislation, (EU Directives 90/313/EEC, later amended by 2003/4/EC), the right to access environmental data improved the public’s insight into environmental information and obliged policy making organisations to heavily invest in environmental planning and enact a broad spectrum of legislative measures.

In every major European city there is some kind of network system for monitoring and mapping the distribution of air pollution and human exposure. These systems generally encompass in-situ air quality monitoring stations, emission inventories, meteorological and air quality modelling, air quality mapping and air quality impact assessment of various control strategies in support of evaluation of action plans. Examples of decision support systems used in major European cities are the IMPAQT (Integrated Modular Program for Air Quality Tools, UK), the Austrian AirWare, the Norwegian AirQUIS, the Swedish EnviMan. The Finnish AQM system is based on integrated dispersion and exposure modelling system allowing for estimation of the spatial and temporal distributions of concentrations and resulting population exposures. In particular, currently for the Greater Athens Area (GAA) there exists one prognostic system for gaseous air compounds only (http://forecast.uoa.gr). At country level, for the whole domain of Greece, there is a forecasting system for gaseous pollutants on a coarse resolution of 10x10 km$^2$ (http://lap.physics.auth.gr/forecasting).

As most of the intensely populated European cities hold a decision support tool for forecasting air quality levels and human exposure, it was deemed necessary to develop such
a tool for the prognosis and assessment of air pollution in the GAA, a region of complex
topography particularly susceptible to accumulation of air pollutants. The present study
is concerned with the operation of a flexible, web-based air quality forecasting system for
GAA, currently under development by the Environmental Research Laboratory (EREL) of
the National Centre for Scientific Research “Demokritos”. The system comprises three
major computational modules and is designed to produce meteorological and air quality
forecasting on a high spatial resolution (1 x 1 km²) and for a 72-hours time horizon with 1
hour time step in advance (Figure 1).

The meteorological predictions are produced by the MM5 (Mesoscale Model 5) (Penn State
University version 3.7.2), which has been parameterized for application to the particular
geographical and climatic characteristics of the Greater Athens Area. Its output is used to
produce high resolution daily air emissions inventories for the main anthropogenic and
biogenic pollutants with 1-hour time step by an in-house built processor named EMIS-
LAB. The meteorological prediction fields in combination with the emissions inventories
are used as inputs to the 3-D atmospheric dispersion and photochemical model CMAQ
(Community Multiscale Air Quality, v.4.6), which produces prognoses for concentrations
of gaseous and particulate pollutants. CMAQ can be employed in particularly when facing
problems that have to do with complex emission patterns, source apportionment, as well as
atmospheric processes which transport and transform pollutants in a dynamic environment.
The analysis of the modelling results is performed via custom made MATLAB© post-
processors and GIS (Geographical Information System) environment in an attempt to
estimate air quality indices and compare them to the current EC and national regulatory
limits.

MM5 and CMAQ models as a forecasting suite have been used extensively over the recent
years in the United States, e.g. [Arnold et al., 2003]. However, there have been very few
applications of this system for cities outside the USA, for example in the UK and Spain,
e.g. [San Jose et al., 2002] and [Sokhi et al., 2006]) and China e.g. [Zhang et al., 2004]).
This is the first time this particular set of models (MM5 and CMAQ) is applied for high
spatial and temporal resolution air quality prognoses in Greece. In addition, EMISLab
provides emission estimates amongst others for fine and coarse particulate matter on a 1 x 1
km² domain. Hence, the originality of this work is established by the online prognosis of
both categories of air pollutants, gaseous and particulate matter, on a high spatial and
temporal resolution.

2. HARDWARE SYSTEM DESIGN

The forecasting model is solved using a distributed memory Beowulf cluster. The cluster
consists of an Intel Core 2 Duo@2.66Ghz PC with 2GB RAM, that serves as a frontend,
and 4 Intel Core 2 Duo @3Ghz compute nodes that solve the computational problem. The PC’s are interconnected using a private Gigabit Ethernet Switch through the TCP/IP protocol. The theoretical performance of this cluster is 48Gflops and the actual measured Linpack performance is approximately 20Gflops.

3. DOMAIN DEFINITION

The MM5 model has been configured with four nested domains, as shown in Figure 2. A description of the domains with regards to the number of cells and discretisation information is provided on Table 1. The outer domain is sufficiently large to take as input meteorological data from the Global Forecast System (GFS – NCEP) in order to provide more accurate lateral boundary conditions. The area of application of the photochemical model CMAQ coincides with the inner domain of MM5 and covers a rather large section of Attica. In the vertical, there are 23 half-sigma layers.

![Geographical description of the computational domains.](image)

**Figure 2.** Geographical description of the computational domains.

<table>
<thead>
<tr>
<th>Domains</th>
<th>Number of cells</th>
<th>Horizontal resolution (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain 1 (outermost)</td>
<td>60 x 60</td>
<td>27 x 27</td>
</tr>
<tr>
<td>Domain 2</td>
<td>54 x 54</td>
<td>9 x 9</td>
</tr>
<tr>
<td>Domain 3</td>
<td>54 x 54</td>
<td>3 x 3</td>
</tr>
<tr>
<td>Domain 4 (innermost)</td>
<td>72 x 72</td>
<td>1 x 1</td>
</tr>
</tbody>
</table>

4. THE MODELLING COMPONENTS

4.1. The Meteorological Forecast

The MM5 mesoscale model has been developed by the Pennsylvania State University (PSU) and the National Centre for Atmospheric Research (NCAR). It is a non-hydrostatic meteorological model and it can be used in cases where high spatial resolution (of a few kilometres) is demanded, as in our case study. MM5 is widely applied for operational forecasting. It has been extensively tested in cases of extreme weather events and over areas of complex topography. As previously mentioned, the model uses input from GFS – NCEP for initial and boundary conditions. In our case study, MM5 (version 3.7.2) has been suitably parameterized for producing the meteorological forecast in the working domain. In Figure 3 the topography and land-cover of the second innermost computational domain is presented. Four two-way nesting domains have been employed to downscale the initial conditions from the NCEP GFS model with cell sizes of 27 – 9 – 3 – 1 km, respectively (Table 1, Figure 2). Thus, a very high resolution weather forecast (1 km²) is produced in the
innermost grid that covers the GAA. The generated meteorological data are used as input to CMAQ.

4.2. The Air-Emissions Model

The in-house EMIS-LAB emission processing tool is used to calculate emissions of air pollutants with a spatial and temporal resolution as required by the atmospheric chemistry model. EMIS-LAB has been developed to process existing inventory data producing an emission inventory of air pollutants with high resolution. It is designed to convert emission inventories that are of annual-total or daily-average temporal character, to any temporal time scale, typically hourly, required by the atmospheric quality models. Additionally, spatial processing is performed calculating emissions values for each model grid cell and model layer for selected sources (e.g. point and aviation).

EMIS-LAB is an integrated dynamic modelling system based on MATLAB. The calculation of the biogenic emissions is dependent on the component BEIS 3.12 (EPA). Emissions from biogenic sources, fugitive dust and anthropogenic activities are treated, incorporating among others the influence of meteorological conditions that are produced from Numerical Weather Prediction models (in this case MM5). Other functionalities of EMIS-LAB include the extensive visualization capabilities, both spatial and in time series mode, allowing the user to obtain a complete overview of the modeling output, facilitating the analysis and assessment of the results. In addition, EMIS-LAB provides correct input format to CMAQ, including the Input/Output Applications Programming Interface (I/O API) and the Network Common Data Form (NetCDF) output format.

EMIS-LAB can process a large number of air pollutants, including toxic gases that are defined by the users. However, its intended application in regional air quality application requires the handling of critical gaseous pollutants such as carbon monoxide (CO), nitrogen oxides (NOx), volatile organic compounds (VOC), ammonia (NH3), sulfur dioxide (SO2) and particulate matter (PM) of different sizes, PM 2.5 and PM10.

4.3. The Air-quality forecast

CMAQ is a complex three-dimensional, (3D), Eulerian numerical air quality model. It is designed as a state-of-the-science “one atmosphere” air quality model involving complex atmospheric pollutant interactions and predicts ambient pollutant concentrations at various scales (regional and urban) in the low atmosphere. The CMAQ system can simulate concentrations of tropospheric ozone, acid deposition, visibility, fine particulate and other air pollutants. The CMAQ modelling system requires 4D meteorological data which are generally provided by a mesoscale meteorological model (in this case MM5). The one-way coupling of MM5 to CMAQ is accomplished through a meteorology–chemistry interface processor MCIP (Meteorology Chemistry Interface Processor) [Byun and Ching, 1999]. The adjoint variation of the CMAQ 4.5 model has been parameterized and applied for the two innermost domains (3x3 km² and 1x1 km², see Table 1) in nested mode. The chemical mechanism incorporated in the system is CB-IV including chemical reactions in the gaseous and liquid phase.

5. CASE STUDY APPLICATION

For the purpose of system testing, a case study for two selected dates February 17 and April 8, 2008 has been simulated. The first date was a particularly cold winter day for Greece, during which the snowfall that occurred was amongst the heaviest snowfalls in the last decade according to the available historic weather reports. The second date was chosen to simulate a business as usual scenario as regards to meteorological and emission conditions.
5.1. Meteorology

The selected parameterization on MM5 was the Grell cumulus scheme, the MRF PBL scheme based on Troen-Mahrt representation, the CCTM2 radiation model, and the simple ice explicit moisture scheme. The number of vertical layers in the modelling study was set to 23, with a telescopic increase with height. The initial data were obtained from the GFS model at the 00:00 run.

The following series of figures yield the various calculated fields of the modelling system (Figure 3 and Figure 4) and present a preliminary comparison of the MM5 output at different domains against experimental observations. Figure 3 shows an MM5 text output referring to the weather forecast of the NCSR D location in Aghia-Paraskevi, for the period from February 17 (Sunday) to February 20, 2008. The model correctly predicted the commencing of the snow fall that started on Sunday midday and lasted until Monday morning. The predicted wind field can be sketched in vector form, an example is shown in Figure 4, from the 3rd modelling domain (3×3 km²), for the 8th of April on 12:00 UTC.

A preliminary evaluation of the model predictions is presented in the following figures. The model output is able to capture accurately the vertical profiles of temperature and relative humidity as it can be deduced from Figure 5. On the 8th of April the model seems to overpredict relative humidity on the highest layers. Concerning the surface wind speed, the comparison was performed against observational data from the Athens International Airport (code LGAV) recorded every hour for that day. The data used in this validation study were obtained from the monitoring network of the Hellenic National Meteorological Service.

Figure 3. Weather predictions in text format.  

Figure 4. Predicted wind field for April 8.

Figure 5. Comparison of vertical profiles of temperature and relative humidity.
5.2. Emissions

The MM5 output was further processed using MCIP to provide the meteorological fields for the emission processing system EMIS-LAB. EMIS-LAB has the ability to rapidly adapt to the particular conditions of that day. On the 17th and 18th of February the entire Greater Athens Area experienced particularly difficult meteorological conditions, which dramatically affected the economic and transportation activity on these specific days. The Athens International Airport was closed during the entire day and shipping was cancelled due to very strong winds. Therefore, the emissions consisted primarily of: (i) the main industries that were treated as point sources, (ii) road-traffic and rail, as the remaining transportation sources, (iii) domestic heating and (iv) biogenic emissions. Each of the above mentioned sources was processed using a suitable and unique temporal (hourly) and chemical profile based on previous studies (Winiwarter et al., 2003) and existing databases (e.g. EPA SPECIATE, SMOKE) so that finally gridded emissions were generated. Moreover, road-traffic was treated taking into account the highly reduced number of vehicles and vehicle speeds for the particular dates. An example is presented in Figure 7, at 11:00 on the 17th February and at the lowest model layer. Figure 8 presents the PM2.5 emissions from nonroad mobile sources and CO emissions from all sources.

Figure 6. Scatter plot of observed and modelled surface wind at LGAV.

Figure 7. Hourly emissions estimate at 12:00, February 17, 2008.

Figure 8. Hourly emissions estimate at 12:00, April 8, 2008.
5.3. Air quality

The MCIP processed output of MM5 on the two finer domains was used as input to the CMAQ in addition to the generated emission file in NETCDF format. As mentioned in Section 2, initially CMAQ was run for DOMAIN 3 and its output was used as initial and boundary conditions to the second run performed in the working DOMAIN 4. Initial and boundary conditions (IC/BC) were also derived from typical profiles of the gaseous species CO, O3, NO2 and SO2 provided with the CMAQ source code, modified to reflect the situation in the area of NCSR, using background observational data. The CB-IV (Carbon Bond IV) chemical mechanism with aerosols and aqueous chemistry was chosen in addition to the Euler Backward Iterative (EBI) for temporal discretization.

![Figure 8. CMAQ output shown for February 17, 2008 in accordance to the national air quality limits set by the Greek Ministry of Environment.](image)

![Figure 9. Comparison of model calculated results for O3 with observations at NCSR station (a) Feb 17, (b) Apr 8.](image)
Figure 8 presents the output of CMAQ for the 17th of February in accordance to the national air quality limits set by the Ministry of Environment. Due to the prevailing meteorological conditions it can be observed that none of the priority pollutants that were examined appear to exceed the national limits. Ozone does not appear to be generated by photochemical reactions due to heavy cloud coverage. Figure 9 depicts the hourly calculated O3 concentrations and the observed values of the pollutants from the NCSRD air quality monitoring station for both days examined. The results show that a relatively good agreement is reached, although further and more thorough model validation is currently under way. Modelling discrepancies in the early hours of the 8th of April are attributed to the initial conditions of the run.

6. Conclusions

The NCSRD air quality forecasting system has been developed by the Environmental Research Laboratory aiming potentially at the assessment of air pollution in the Greater Athens Area. The system is an integrated modelling framework comprising the: (i) MM5 meteorological model, resulting in a very fine resolved domain for Attica (1 x 1 km²), (ii) EMISLAB, a dynamic anthropogenic and biogenic emission processing model, (iii) CMAQ, which is the state-of-the-art photochemical model and (iv) extensive post processing options for visualization and more user friendly presentation of the results.

As a test case, the 17th of February 2008 was studied and a primary evaluation of the modelling components against observational data from the existing monitoring networks was presented. This work represents the first application of the MM5-CMAQ system in Greece for predicting air pollution levels. Future work will include sensitivity studies of the air quality predictions to the emission inventories.

ACKNOWLEDGEMENTS

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