An Operational Model for Air Qualityimulations in the Campania Region

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1 Introduction

Air quality models are used as the most powerful and the only scientifically relevant tools for identifying effective strategies to improve air quality. In the past, eulerian chemical transport models have been successfully used to simulate pollutant dynamics over many urban areas. This kind of studies were aimed at providing guidance to air quality management agencies; many European countries and local administrative authorities used computer simulations as basic support of their environmental policy.

In this report we describe the design of a limited-area operational air pollution model. This software has been primarily intended for policy applications on the Campania Region (in Southern Italy). It has been designed to run on heterogeneous parallel systems.

During the last years, many national and local environmental protection agencies have been developing and testing increasingly complex model to address air pollution problems. The aim of this work was usually to assess, through the use of such models, the cost-effectiveness of environmental regulatory acts. Following that trend, the Office of Scientific Research and the Environment Office of the Campania Regional Board (Campania is one of the Italian's regions) recently funded a research program for developing an operational model. This model covers some aspects of air pollution modeling application, namely scenario simulations, episodic studies, monitoring and forecasting for a short time scale. Moreover, since recent advances in computer technologies allow the redesigning of air pollution models, the Regional Offices strongly encouraged the use of advanced parallel computers. Our software has been targeted for a Beowulf parallel computer.

This activity has been carried out at the Center for Research on Parallel Computing and Supercomputers (CPS-CNR), in Naples, by an interdisciplinary team of atmospheric chemists and computational mathematicians.

2 System components

The system consists of three main, uncoupled, subsystems: the meteorological driver, and emission pre-processing model and a chemical transport model, respectively. All the subsystems have been embedded in a computational framework, whose main function providing integration among the different components and a user-friendly interface.

The meteorological subsystem is the public domain software MM5-V3 (the fifth-generation Mesoscale Model, version 3, Dudhia *et al*. 2001). It has been widely used by many research and institutional centers as an operational tool for weather forecasting. MM5 provides the three-dimensional fields of the wind velocity vector, temperature, pressure, friction velocity, etc. The wind velocity vector is used to predict the mean transport of chemical pollutants in the modeling domain; temperature and pressure provide quantitative information on the stability of the atmosphere and allows one to estimate mixing heights, turbulent diffusion coefficients and the kinetic rates of chemical pollutants.

Initial and boundary conditions are generated from data of ECMWF center (European Center for Meteorological Weather Forecasting) using objective techniques.

An emissions inventory has been historically defined as a compilation of emissions data and descriptive information for sources of air pollution over the Campania region. With few exceptions, emissions inventories developed for regional air quality studies are based on an emissions model. The activity level or throughout, can be defined as a measure of production rate, fuel consumption, or another indication of source activity levels (e.g., tons of fuel burned). An emission factor is an emission rate used with an activity level or throughput rate to estimate emissions. Emission factors are determined by measuring emissions, usually from more than one source within a source category, under varying conditions. For the present study we used the Corinair suggested emission factors. The emissions model comprises numerous sub-models for estimating emissions for each source category, and for spatial disaggregation, temporal allocation, chemical speciation, and size classification of emitted pollutants.
Emissions have been estimated for the Campania region during 1995. Estimates have been specified using activity levels and emission factors for the following sectors:
Road traffic
Biogenic emissions

Currently we are at work to estimate emissions from residential heating and industrial combustion and processes for 1995. The sub models account for emissions of total organic compounds (VOCs), NO_x and CO.

A commercial Geographical Information System (ArcView™) and the public domain Vis5D (Vis5d, 1999) software has been employed for emission data processing and visualization (either of input and output data).

The chemical transport model (that we named PNAM) is based on an eulerian approach, i.e. solves the continuity equations, defining the time evolution for each chemical compound (42 compounds). The continuity equation is expressed in the following form:

$$\frac{\partial C_i}{\partial t} = -u \cdot \nabla C_i + \nabla \cdot \left(K \cdot \nabla C \right) + E_i + D_i + R_i \qquad i = 1, N$$

This equation takes into account the primary emissions, the dry deposition, the effect of transport and dilution due to wind and the photochemistry. We have not taken into account cloud/fog physics, aerosol physics and chemistry, aqueous phase chemistry, wet deposition The total duration of a simulation is of the order of some days (the typical duration of a photochemical smog event).
Since the identification of the most effective reduction strategy may encompass a large number of simulation, computers equipped with parallel architecture were used. Parallelism was introduced into PNAM by a two-dimensional grid partitioning, cutting the computational domain along the *x*- and *y*-directions. The application of a dynamic load balancing strategy, where a load balancing algorithm is executed periodically to determine a new and more balanced data partitioning among available processors, allowed to get efficiency and scalability. PNAM has been designed to run over multiple active nests; this allows to get better resolution over predefined areas (e.g. urban areas). Currently nesting implementation is static, uniform and one-way.
The RSL (Runtime System Library, Michalakes, 1997) was employed for domain decomposition and refinement, local address space computation, distributed I/O and interprocessor communication. RSL is the interface between PNAM and the low-level message-passing library MPI (Gropp *et al*., 1999).
Parallel performances has been tested on Beowulf machines and IBM SP machines.

The system has been embedded into a computational framework which consists of an interface between the user and the system, as well as a set of low-levels modules for managing data exchange

among the various components. Major functions were embedded in three specialized components: the *data manager*, the *strategy manager* and the *system monitor*.
The *data manager* provides the interface between the various subsystems. It will typically perform internal data exchange, internal import and export, and file format conversions. Moreover it will allow access to experimental data gathered by the Environmental Office at the Campania Regional Board.
The *strategy manager* is designed for supporting non-specialist end-users in describing, designing, executing and analyzing an air quality simulation. Using this tool, the user will be able to perform a "what if…?" analysis, by changing landuse parameters, emission factors, initial and boundary conditions, photolysis rates, etc. The strategy manager is also able to store and retrieve large data collection of simulations from the system database. The extent and flexibility and effectiveness in the analysis of input and in the interactive exploration of simulation results is a critical issue in the design of the strategy manager component.
The *system monitor* provides supervising and state tracking capabilities on the execution of different software components.
Preliminary results have been published elsewhere (Barone *et al*., 1999, 2000). The chemistry/ transport component was able to simulate the gross feature of photochemical dynamics over the Campania region, though some discrepancies were evident. We are currently at work to improve the emission inventory and to achieve better performance on parallel computers.

3 Conclusions

During the last year, activities have been devoted to the implementation of a modeling framework to study air pollution problems over the Campania region. Our strategy has been based on the integration of well-known software for the simulation of meteorological scenarios, and data analysis and visualization. The design of the modeling system includes a meteorological driver (MM5), an emission model and a chemical transport model. A graphical user interface allows data display and analysis and a rapid "what if" analysis.

The system has also been designed to run on advanced, low cost, easy to use, parallel computer, namely a cluster of PC's, that can be reasonable implemented and operated even at a small, local environmental office.

We have followed a rather conservative approach in designing this system. Many advanced features will not be included in this system, mainly in the science behind the chemical transport model and the emission model, for instance aerosol chemistry, wet deposition, higher-order closure for turbulent transport, etc. The very reason for such a choice is that we are aware that there is a serious lack of data for the Campania Region. This prevents a reliable simulation or parameterization of many chemical and physical processes. In the coming years our aim is provide the local environmental Authority and the scientific community with an improved operational tool.

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