PROCEEDINGS OF SCIENCE

Porting the WRF Model to EumedGrid and Simulation of Air Quality in Urban Zones

Chaker El Amrani
Abdelmalek Essaadi University
FST, PO. Box 416, Tangier, 90000, Morocco
ch.elamrani@fstt.ac.ma

The Weather Research and Forecast (WRF) is a specific program for forecasting and research. WRF processing is composed of three steps: pre-processing, core model execution and post-processing.

WRF/Chem is the WRF coupled with Chemistry. The model simulates the coupling between atmospheric dynamics, radiation and chemistry, and is used for investigation of regional-scale air quality, field program analysis, and cloud-scale interactions between clouds and chemistry. WRF/Chem can predict transport of atmospheric constituents and radiation of O_3 and UV.

The WRF/Chem processing requires high execution time and storage space. The porting to Grid Computing can be very advantageous since the model supports hybrid distributed and shared memory computations.

The Grid platforms used for this study are MaGrid and EumedGrid. MaGrid is linked to EumedGrid, and users can have access to appropriate CPU and storage resources. The Grid Computing abundant resources enable multiple scenarios to run in parallel, and the MPI parallel programming model allows execution time to decrease substantially with increasing the number of Worker Nodes. In addition, for most scenarios' simulations, numerical grid can be more refined especially in sensitive regions, leading to a higher degree of accuracy in the results.

In this study, the WRF/Chem is ported to Grid computing, and is used to simulate emissions of pollutants in the North of Morocco.

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1. Introduction

The main objective of this study is to simulate air quality in urban zones in Morocco, using WRF/Chem model, and Grid Computing technology.

The World Health Organization defines air pollution as the contamination of the indoor or outdoor environment by any chemical, physical or biological agent that modifies the natural characteristics of the atmosphere [1].

In major cities in Morocco, rapid urbanization, burning of fuel, release of chemicals and density of maritime traffic have resulted in increasing urban air pollution. Several pollutants, such as carbon monoxide, ozone and sulfur dioxide are of major public health concern.

The WRF/Chem can simulate air pollution. It is an intensive processing and data application that requires large scale computing and data resources. In this study, WRF/Chem will be ported to Grid Computing, and several air pollution scenarios in Morocco, based on biogenic and anthropogenic emissions, will be simulated.

This work has been conducted in collaboration with the Italian Research Council Institute for Amospheric Pollution (Rende Section), in Italy.

2. Urban Air Pollution

The Air pollution problems on the Earth are as old as Earth itself. But recently it increased due, among others, to rapid urbanization, burning of fuel and release of chemicals. Urban air pollution is estimated to cost approximately 2% of GDP in developed countries and 5% in developing countries [2].

Pollution problems include urban smog, indoor air pollution, acid deposition, global ozone reduction, and global warming.

Air pollution is due to biogenic, geogenic and anthropogenic emissions. The biogenic emissions come from natural sources, such as vegetation and soils. The geogenic emissions are caused by non-living world, such as volcanic emissions, sea-salt emissions, natural fires and desert dust. And the anthropogenic emissions come from human activities, such as burning fossil fuel.

Pollutants are classified as primary and secondary substances. The primary pollutants are substances emitted from sources. The main primary pollutants known to cause harm in high concentrations are Carbon, Nitrogen and Sulfur Compounds, such as: carbon dioxide (CO_2), ammonia (NH_3) and sulfur dioxide (SO_2).

Secondary pollutants are formed in the atmosphere from primary pollutants. Nitrogen dioxide (NO_2) and Ozone (O_3) are examples of secondary pollutants of major public health concern when concentrations in the atmosphere are high.

Air pollution causes a variety of human health effects especially on children, among others: respiratory infections, asthma, allergies and neurodevelopmental diseases.

3. Air Pollution Modeling

Air pollution modeling can provide a complete description of the air quality problem. It is used to describe the variability in space and time concentrations of substances in the atmosphere according to four general types of processes: emissions, transport, chemistry, and deposition.

These numerical models solve the continuity equations for mass conservation of the chemicals in the atmosphere. Simulations are based on mathematically representing emissions and the local meteorology such as sunlight, wind, and temperature.

There are two different modeling approaches, Lagrangian modeling and Eulerian modeling.

These models are essential to gain understanding about the behavior of various compounds in the atmosphere, and to evaluate control strategies aimed at reducing pollution to meet air quality goals [3].

4. The WRF/Chem Model

The WRF/Chem model is released as part of the Weather Research and Forecasting (WRF) modeling package. It is developed by an international community, and leaded by the National Oceanic and Atmospheric Administration (NOAA) / Earth System Research Laboratory (ESRL) [4,5].

WRF/Chem model can simulate chemistry and aerosols, and have the option to simulate the coupling between dynamics, radiation and chemistry. Uses include forecasting chemical-weather, testing air pollution abatement strategies, planning and forecasting for field campaigns, analyzing measurements from field campaigns and the assimilation of satellite and in-situ chemical measurements [5].

Biogenic emissions can be included in WRF/Chem by online calculation of biogenic emissions, online modification of user specified emissions or by online calculation from MEGAN [6,7].

The anthropogenic emissions can be included by user-specified emissions provided in the proper WRF data file format, or by global emissions data from the one-half degree RETRO [8] and ten degree EDGAR [9] data sets.

The WRF/Chem includes as well choices for photolysis and aerosol schemes, and a plume rise model to treat the emissions of wildfires [6].

WRF/Chem has a very modular approach. The chemistry subdirectory has been implemented in version of HIRLAM [10], and is being implemented now into FIM global model [11].

WRF/Chem can simulate release and transport of constituents, and processes that are important for global climate change issues, such as aerosol direct and indirect forcing.

As shown in “Fig. 1”, the WRF/Chem modeling system consists of three major components [6]:

- The WRF Pre-processing System (WPS).
- WRF/Chem solver.
- Post-processing and visualization tools.

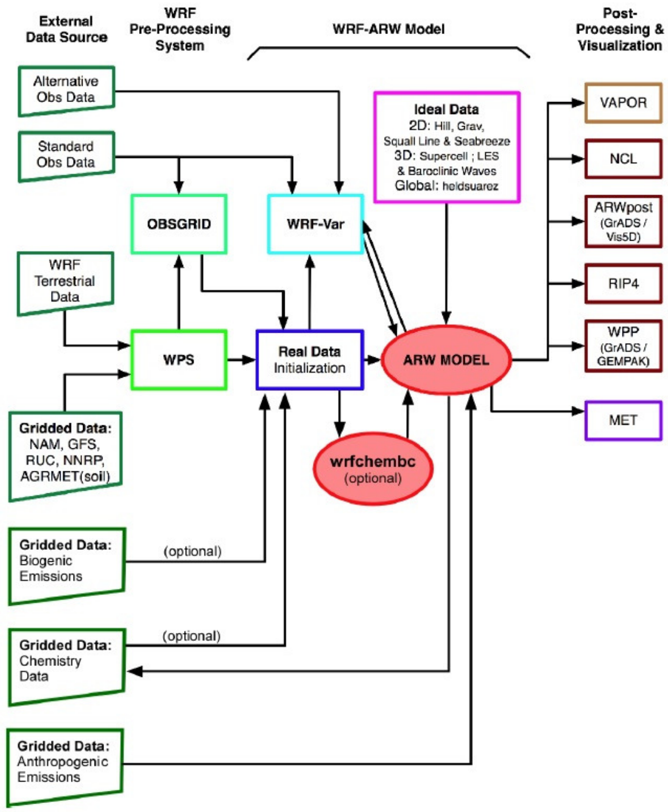

Figure 1. WRF-ARW Modeling System Flow Chart

5. The WRF/Chem Processing

5.1 The WRF/Chem Input

The WRF/Chem includes biogenic and antropogenic emissions, photolysis and aerosols. Namelist.input file, which resides in the same directory as wrf.exe, contains lists of parameters and their values. These determine the model behavior. For instance, if bio_emiss_opt = 1, biogenic emissions will be calculated online using the Gunther scheme.

The anthropogenic emissions can be downloaded from sources such as EMEP (European Monitoring and Evaluation Programme), and the biogenic emissions can be calculated online or from models such as MEGAN (Model of Emissions of Gases and Aerosols from Nature).

5.2 Modeling Domains

The Domain can be modeled using the WRF Portal, which is a graphical user interface (GUI) front end for selection and localization of the domain as shown in “Fig. 2”, running WRF post-processing and visualization of the model’s output. It is written in Java and is portable to all platforms [12].

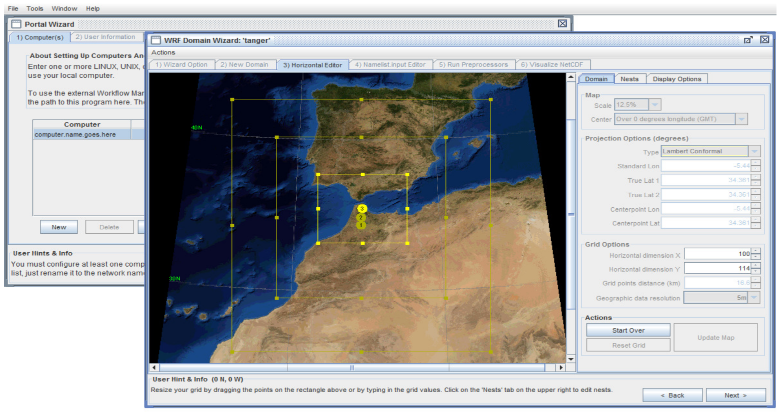

Figure 2. WRF Portal Domain Wizard

5.3 WRF/Chem Pre-processing

The WRF Pre-processing System (WPS) is composed of three programs:

- geogrid: defines the simulation domains, and interpolates terrestrial data sets to the model grids.
- ungrid: "degribs" the data, and writes the data in a simple format, called the intermediate format.
- metgrid: horizontally interpolates the intermediate-format meteorological data that are extracted by the ungrib program onto the simulation domains defined by the geogrid program.

The program prep_chem_sources provides biomass burning, wildfire, and anthropogenic emissions to the WRF/Chem forecast [6].

During this phase, bash scripts will retrieve data from appropriate sites. The environmental variable WRF_CHEM must be set to 1.

5.4 Processing and Postprocessing Phases

The processing phase consists on configuration based on computers' architecture and programming model: sequential, shared or distributed memory, compilation and execution of the WRF/Chem binaries. The simulations' run-time on a given hardware architecture depends on the nested domains and the grid resolution.

The WRF/Chem outputs are visualized and analyzed with tools like ncview, NCL and VAPOR [13,14].

6. Porting WRF/Chem to Grid Computing

The WRF/Chem is an intensive processing and data application. The porting of WRF/Chem to Grid Computing is very advantageous as the Grid infrastructure can provide the required computing resources and storage space [15]. Moreover, the execution of WRF/Chem on the Grid can be distributed and/or shared memory based.

The Grid Computing infrastructures used in this study are EumedGrid [16] and MaGrid [17].

EumedGrid is a Grid Computing initiative setup by EGEE collaboration. It serves the Mediterranean region as a pilot grid infrastructure for research. EumedGrid is interoperable with the EGEE [18], the European infrastructure, as well as with other similar grid initiatives. It supports 25 sites across 13 Mediterranean countries.

MaGrid is representing the Moroccan grid infrastructure [19]. Its clusters are made available to the computing and storage needs of Moroccan and Mediterranean Universities and Research Centers [20]. MaGrid is connected to EumedGrid, and is located and administered in the National Center for Scientific Research and Technology (CNRST). It has been operational since 2005. The CNRST has established a Certification Authority named MaGrid CA in 2007.

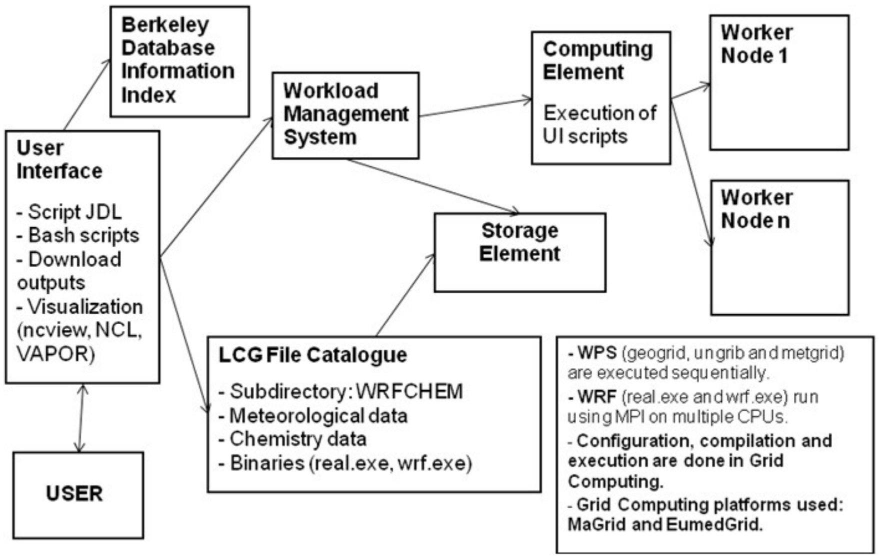

Figure 3. Overview of WRF/Chem on the Grid

The WRF/Chem is implemented in Grid according to the design shown in “Fig. 3”. Simulations are executed in the closest Computing Element with MPICH2 installed, MPI Shared Home and Free CPUs. The MPI Shared Home option lets the file be compiled in one Worker Node, and be read by the other Worker Nodes in the same site. The Virtual Organization used is “Eumed” which provides substantial software and hardware resources.

Shell scripts are written to define the BDII (Berkeley Database Information Index), the LFC (LCG File Catalogue) and other User Interface sub-directories. Several WRF/Chem files are copied to a Storage Element, and registered in the catalogue. The files are downloaded from the Storage Element to the Computing Element.

Several parameters are defined in the JDL file, such as the required number of processors and the preferred Computing Element. When the simulations are done, results are packed and uploaded to the User Interface. NCL, VAPOR and ncview software, installed in the User Interface serve to analyze and visualize the model outputs.

To use the Grid Computing resources, a short term proxy and a long lifetime proxy had to be setup and retrieved from the WMProxy server.

The JDL job includes the sequential execution of WPS programs: geogrid, ungrib and metgrid. The MPI WRF/Chem execution starts when compilation is successful.

Domains are defined and localized by selecting a region of the Earth and choosing a map projection. Information is stored in namelist.wps and namelist.input files. The first one is used by WPS, and the second by WRF.

The Grid Computing abundant resources enable multiple scenarios to be executed in parallel, and the MPI parallel programming model allows execution time to decrease substantially with increasing the number of Worker Nodes.

7. Applying WRF/Chem to North of Morocco

Morocco's extractive industries are potentially highly polluting, and pollution issues also arise in the petroleum refining, food processing, and cement and textiles industries. These produce a range of solid wastes and effluents, including hazardous wastes [21].

The origin and the percentage of emissions in urban zones in Morocco are as follow: energy 56%, agriculture 25%, Forest 7%, industry 7% and waste 5%.

A correlation has been found between air pollution and health needs in a number of cities. Mortality, for instance, has increased by 2% due to the increase of PM10 concentrations by 22µg/m3 [22].

"Fig. 4" shows the ozone concentration in the Mediterranean basin [23]. The density of maritime traffic in the Gibraltar Strait is considered as one of the highest in the world. This has direct impacts on the air quality of the northern cities of Morocco.

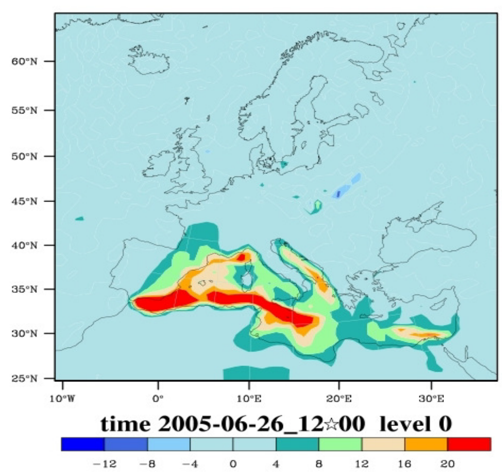

Figure 4. Ozone Concentrations in the Mediterranean Basin due to the Shipping Traffic

Ozone can cause Irritation of the respiratory system, causing coughing, throat irritation, and/or an uncomfortable sensation in the chest. Also, ozone makes people more sensitive to allergens, which in turn trigger asthma attacks.

In this study, The WRF/Chem is used to simulate the biogenic and anthropogenic emissions in north of Morocco.

This investigation can help Moroccan decision makers to analyze air quality scenarios and make decisions based on the model outcomes.

8. Results

Simulations are conducted for the north region of Morocco. The model's outputs represent the simulated emissions on November 1st, 2011.

The User Interface is a MaGrid machine, and the rest of the machines are from both MaGrid and EumedGrid platforms. A single Worker Node has a quad-core processor.

The simulations run on different number of CPU in order to evaluate the performance of the Grid Computing plateform.

The emissions of several pollutants are predicted by the WRF/Chem, based on initial and boundary conditions of meteorological data, biogenic and anthropogenic emissions. Every six hours results are obtained, and new observational data are input into the model.

Ozone, Ammonia and Formaldehyde concentrations in the North of Morocco are represented in the following figures.

The WPS runs in sequential mode, while the execution of WRF/Chem is in parallel on multiple processors and distributed memory. Consequently, a WRF/Chem job is divided into several tasks, each of them is dispatched to an available worker node. The program outputs are stored in the storage element.

From "Fig. 5", it can figure out that the run-time of the model decreases when the total number of processors used during the simulations increases. This result is satisfactory since the overall progress shows that we have gained speedup. According to this figure, only 28.6% of the run-time measured with one CPU is needed when the CPU number is twenty. The Grid Computing has enabled a substantial reduction in the execution time.

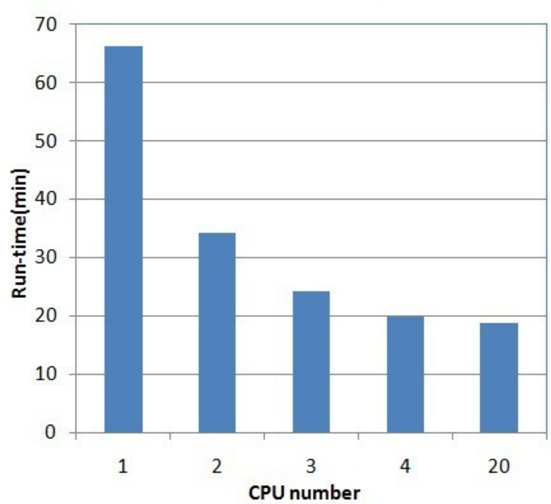

Figure 5. Run-time vs CPU number

"Fig. 6" shows high ozone (O_3) concentrations nearby the Atlas Mountains, these regions are close to several industrial zones in Casablanca, and to the petrol refinery located in Mohammedia. The ozone emissions are released by these plants, and pushed by winds across these regions.

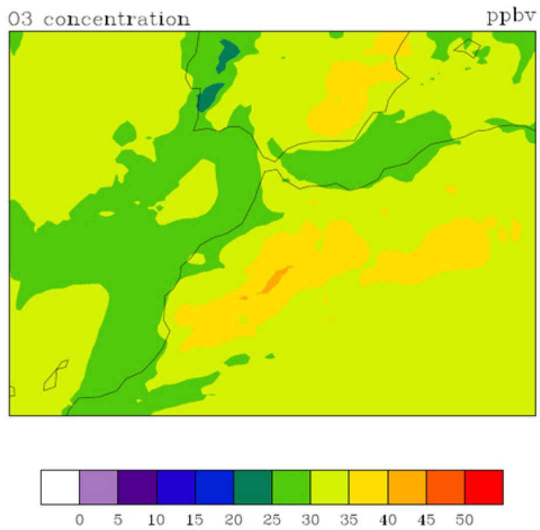

Figure 6. Ozone Concentration

Ammonia (NH_3) is mainly emitted by agricultural processes, farming activities and use of pesticides and fertilizers. "Fig. 7" shows high concentrations of Ammonia in the north-west of Morocco, especially in the Gharb plain, a favourable region for farming and agricultural activities.

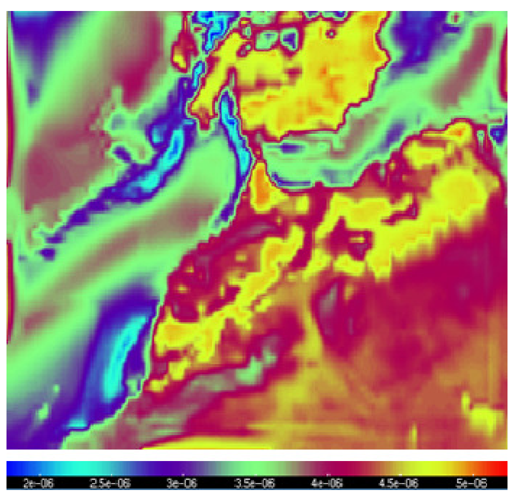

Figure 7. Ammonia Concentration

The Formaldehyde (HCHO) is a chemical used in industry. It is also produced during burning of organic material. The Formaldehyde plays an important role in ozone formation. In "Fig. 8", Formaldehyde levels are highest in the northen cities. These regions have experienced over the last years a dramatic increase in urbanization. In addition, the progress of industrialization has also grown. This has accelerated the development of these areas, but has negatively affected the air quality.

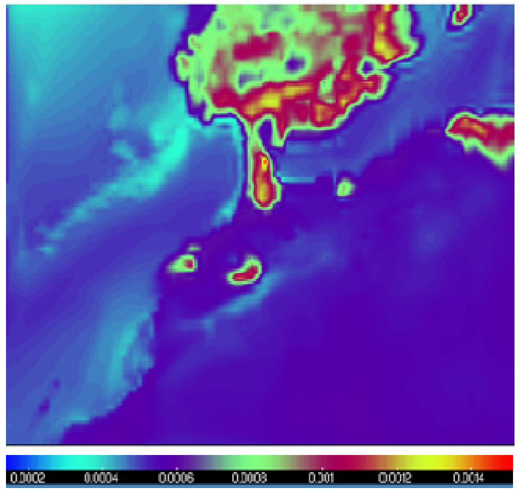

Figure 8. Formaldehyde concentration

The above figures represent the emission of three gases due to industrialization, agriculture and urbanization. More scenarios analysis on refined domains will allow assessing other air pollutants emissions.

9. Conclusion and Future Work

In this study the WRF/Chem has been successfully implemented in MaGrid and EumedGrid, and several bash scripts for downloading meteorological and emissions data, and managing jobs' workflow have been developed.

The model simulations of main biogenic and anthropogenic emissions in the north of Morocco have been conducted, and showed high concentrations of Ozone, Ammonia and Formaldehyde in some regions of the country.

The use of Grid Computing technology and parallel programming model MPI has resulted in optimizing the run-time of WRF/Chem execution.

Future work aims to using OpenMP parallel programming model together with MPI, in order to take profit from the multi-core CPU architecture of worker nodes, and accelerate the model execution. Also, several intensive processing subroutines of WRF/Chem will be ported to Graphics Processing Unit (GPU) to increase the speedup.

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