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NEAR REAL TIME EVALUATION OF THE SPANISH AIR QUALITY FORECAST SYSTEM: CALIOPE

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Abstract: The most recently adopted European Directive on Ambient Air Quality and Cleaner Air For Europe (Dir. 2008/50/EC) promotes the use of air quality models to provide geographically distributed information about air quality levels. It also quantifies the modelling uncertainty objectives for the regulated pollutants (O3, NO2, SO2, PM10 and PM2.5 among others) Therefore it is fundamental to establish the reliability of the currently used models to help decision makers and final users.

The WRF-ARW/HERMES-EMEP/CMAQ/BSC-DREAM8b modelling system provides high resolution air quality predictions for 48h in Europe –EU12- (12x12 km2, 1h), the Iberian Peninsula and Balearic Islands –IP4- (4x4 km2, 1h) and Canary Islands –CAN2- (2x2 km2, 1h) since July 2007, under the framework of the CALIOPE project (Baldasano et al., 2008; http://www.bsc.es/caliope/). A near real time evaluation system has been developed and it is on-line and in operation since January, 2009. Non validated near real time air quality data from more than 400 surface stations are compared to ground-concentration predictions in Spain. Seven ozonosondes are used to test the performance of the model in reproducing O3 vertical structures in Europe, Spain and Canary Islands. Additionally, OMI images are used to qualitatively assess the vertical column densities of NO2 predicted for Europe.

The CALIOPE modelling system proved to have good skills in predicting the gaseous pollutants levels (O_3, NO_2 and SO_2), although it slightly underpredicts PM_{10} and $PM_{2.5}$ concentrations, hence some of the on-going works and developments focus on this issue. Moreover, a complete evaluation for the 2009 season against validated observations is planned.

Key words: air quality modelling, forecast, evaluation, near real time.

INTRODUCTION

According to the last EU Directive on Ambient Air Quality and Cleaner Air For Europe (Dir. 2008/50/EC) air quality modelling is a useful tool to understand the dynamics of air pollutants, to analyze and forecast the air quality, and to develop plans reducing emissions and alert the population when health-related issues occur. This Directive sets also the limits for human health protection for significant ambient air pollutants, such as O_3, NO_2, SO_2, PM_{10} and $PM_{2.5}$, and provides a measure of the desired uncertainty levels to be achieved by modelling techniques. The assessment of the reliability on model predictions is fundamental to help decision makers and provide a feedback to general public.

A high-resolution air quality forecasting system, namely WRFARW/HERMES-EMEP/CMAQ/BSC-DREAM8b, has been developed and applied to Europe (EU12: 12 x 12 km^2, 1hr) as well as to Iberian Peninsula (IP4: 4 x 4 km^2, 1hr) and Canary Islands (CAN^2: 2x2 km, 1hr), in the framework of the CALIOPE project (Baldasano et al., 2008a). The modelling system has been implemented on the MareNostrum supercomputer, hosted by the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS), which allowed the high resolution simulations.

The forecast model, in operation since July 2007 and available online at www.bsc.es/caliope, predicts the concentration of gaseous pollutants (O_3, NO_2, CO, SO_2) and particulate matter (PM_{10}, $PM_{2.5}$) during 48 h for the domains of study. The main goal of this paper is to describe the Near Real Time evaluation system implemented online and to assess the overall behaviour of the CALIOPE modelling system in the forecast mode.

METHODS

The Near Real Time (NRT) evaluation system has been developed to compare the model results with regard to the observations. This section describes the modelling system and its setup, and then the definition of the atmospheric observations used is provided.

Modelling system

CALIOPE is a state-of-the-art modelling framework constituted by several models, which has been extensively evaluated in the diagnostic mode (Baldasano et al., 2008a; Jiménez-Guerrero, 2006, 2008a; Piot et al., 2009; Pay et al., 2009, 2010). The degradation of the meteorological predictions with time in a forecast mode (without applying data assimilation corrections) is a well-known issue (Honoré et al., 2008). Therefore, in the model evaluation the D+0 (first 24 hours of simulation) and D+1 (24 to 48 hours of simulation) are independently treated.

The Advanced Research Weather Research and Forecasting (WRF-ARW) Model v3.0.1.1 (Skamarock and Klemp, 2008) provides the meteorological inputs for the simulations. The defined domains cover Europe (EU12: 478x398 cells, 12 km, 1 hr resolution), the Iberian Peninsula (IP4: 397x397 cells, 4 km, 1hr resolution) and Canary Islands (CAN2: 202x302 cells, 2 km, 1 hr resolution). The meteorological simulations consider 38 vertical σ-levels and 50 hPa as the top of the atmosphere. The boundary conditions for the inner domains are obtained from the EU12 simulation. The NCEP/GFS GRIB2 model (at 0.5º) is used for the initialization of the model.

The emissions is made by the High Elective Resolution Modelling Emission System (HERMES; Baldasano et al., 2008b). For the European domain the 2004 EMEP emissions database is used, and HERMES disaggregates this information taking into account activity data and land cover uses, in a top-down approach. HERMES is applied to Spain following a bottom-up methodology, and the estimates of IP4 and CAN2 emissions consider mobile (on-road, ships and planes transport), industrial and power plants, domestic and commercial fossil fuel consumption, solvents use and biogenic emissions. It provides hourly concentrations of gaseous and particulate matter in the adequate resolution and speciated for being used by the CBIV chemical mechanism within Models-3 Community Multiscale Air Qualtiy (CMAQ) model, version 4.5 (Byun and Schere, 2006).

The CMAQ simulations take into account gas phase chemistry, heterogeneous chemistry and sea salt emissions (aero4 module). The initial conditions are obtained from the previous day simulations and the boundary conditions for the outmost domain are based on the LMDz-INCA global model (Szopa et al., 2009) outputs. The vertical resolution applied accounts for 15 σ-vertical layers up to 50 hPa (top of the atmosphere).

The Dust Regional Atmospheric Model (BSC-DREAM8b) predicts the atmospheric cycle of mineral dust (Nickovic et al., 2001; Pérez et al., 2006). BSC-DREAM8b is forced by the NCEP/Eta meteorological driver and it provides mineral dust levels with a 50 x 50 km resolution for the Euro-Mediterranean region. An off-line coupling is applied to the calculated concentrations of particulate matter from CMAQ (Jiménez-Guerrero et al., 2008b)

Observations
One of the fundamental steps in the NRT model evaluation is the collection and treatment of observations. The CALIOPE evaluation system takes into account:

1. Meteorological observations
The system hourly collects and processes wind speed, wind direction, temperature, dew temperature, and mean sea level pressure data for 254 METAR stations covering the EU12 domain and for 88 in the IP4 and CAN2 domains.

2. Ground level concentrations
Hourly ground level concentration data from different air quality networks are used by the CALIOPE evaluation system. The NRT evaluation at ground level takes into account the type and environment of the station, in order to consider data representative of the model scale (e.g. no urban traffic stations were selected in EU domain, because the model resolution in that domain is 12x12 km^2 and the representativeness of these kind of stations varies from 100 m to 1 km, according to the EC Dir. 2008/50/EC). According to that, 3668 background stations are included in the EU12 domain (see **¡Error! No se encuentra el origen de la referencia.**(a)), provided by the European Environmental Agency (EEA, http://www.eea.europa.eu/maps/ozone/resources/about-the-data), which mainly measures O_3 concentration, but in some cases also NO_2, SO_2 or PM_{10}. The IP4 domain accounts for 478 air quality stations and the CAN2, for 34 (**¡Error! No se encuentra el origen de la referencia.** (b),(c)), measuring O_3, NO_2, SO_2, PM_{10} and occasionally $PM_{2.5}$. The Environmental Departments of Andalucia, Catalonia and Canary Islands and the EEA are the current observations providers.

3. Ozonesondes
The World Ozone and Ultraviolet Radiation Data Center (WOUDC), from Environment Canada, provides vertical ozone profiles for five locations in the EU12 domain, including one in Madrid-Barajas (which allows also the evaluation of the IP4 domain profiles). Moreover, the Izaña Atmospheric Research Center (from the Spanish Meteorological Agency – AEMET) supplies an ozone vertical profile from their station in Santa Cruz de Tenerife. The frequency of the measurements varies depending on the station. Usually the profiles they have a weekly frequency.

4. NO_2 tropospheric column data
Daily NO_2 tropospheric column images from AURA - OMI (as processed by Koninklijk Netherlands Meteorological Institute - KNMI) are compared to model predictions in the European domain.

Near Real Time evaluation tool
The NRT evaluation tool is an on-line system (www.bsc.es/caliope) that compares hourly/daily observations with model outputs. It has to be noted that model raw outputs are used, with neither post processing, nor adjustments.

The use of NRT data is subjected to several considerations that may affect the evaluation results. The data obtained from air quality stations are non validated, therefore some stations may present unexpected trends due mainly to lack of maintenance tasks, ambient concentrations below the detection limits (which in case of SO_2 measurements is quite frequent). These aspects are taken into account for the discussion of the evaluation results, although non filtering or observations treatment is currently applied.

As aforementioned, the type and environment of the ground-level stations is taken into account (urban, suburban or rural stations, and traffic, industrial or background environments) in order to select those appropriate for the model scales. The

CALIOPE evaluation system currently includes only background stations in the European domain (12km cells) and all kind of stations for the Iberian Peninsula and Canary Islands (4 km and 2 km resolution cells, respectively).
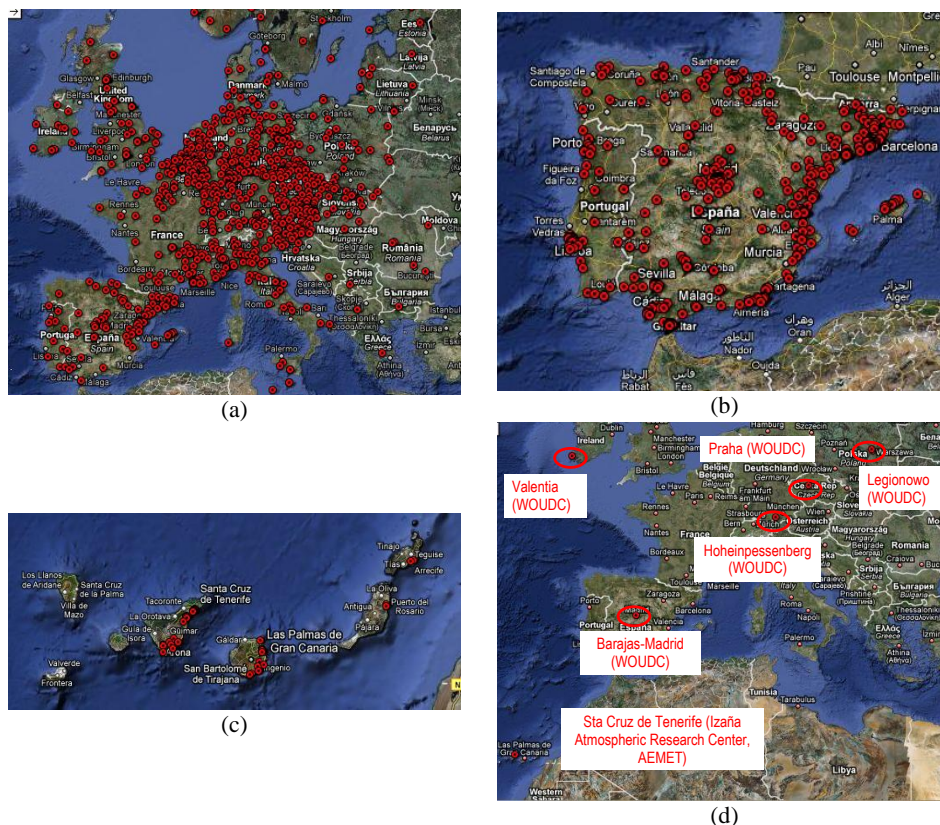

Figure 1. Air quality stations included in the CALIOPE NRT evaluation sytem for the EU12 domain (a), IP4 domain (b) and CAN2 domain (c); and location and responsible agencies for the ozonesonde data in the EU12, IP4 and CAN2 domains (d).

RESULTS AND DISCUSSION

Taking into account the aforementioned considerations, the IP4 and CAN2 evaluation results are discussed in detail.

The ground-level concentration of NO_2 is well captured by the model. Both dynamics and emissions are well characterized by the CALIOPE modelling system, the road network of densely populated areas (more than 500.000 habitants) is explicitly included in the HERMES emission model, therefore a good characterization of the traffic derived concentrations is observed even at urban traffic stations in big cities (Figure 2, left).

CALIOPE predicts the O_3 daily maxima adequately, especially in areas with high NO_x emissions (e.g. urban areas, see Figure 2, right), although a slight underestimation of the nocturnal minimum values is observed. In rural background areas the daily O_3 cycles are fairly reproduced by the model, which suggests that the photochemical model behaviour has to be improved in areas with low NO_x emission levels.

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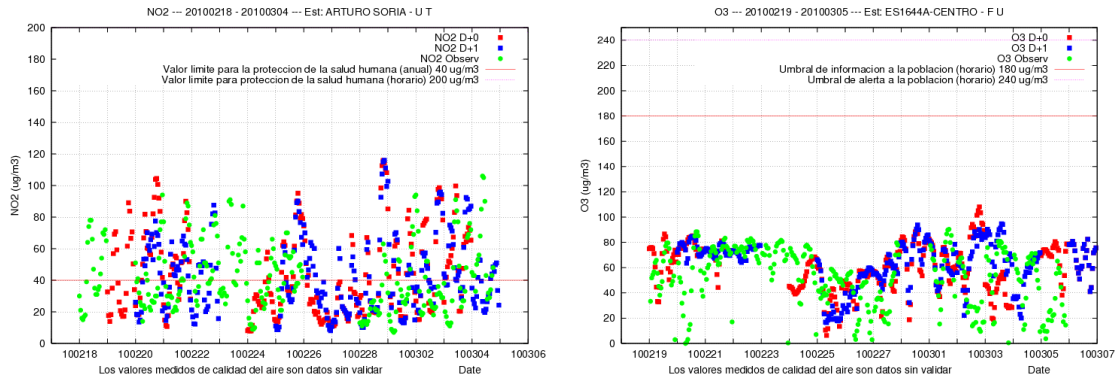Paris, France, 1- 4 June 2010

Figure 2. (Left) Hourly NO_2 concentration as predicted by the CALIOPE system for D+0 and D+1 against observed NO_2 from an urban traffic station of Madrid. (Right) Hourly O_3 concentration as predicted by the CALIOPE system for D+0 and D+1 against observed O_3 from an urban background station in Seville

Mainly due to the regulations affecting the sulphur content in fossil fuels enforced during last decades, the SO_2 levels in Spain have been notably reduced. Nowadays, the observed levels are far below the European targets for human health protection (125 µg m^{-3}- 24 hr mean). In some areas, they are even below the detection limit of the air quality stations and flat profiles are provided by those (e.g. Figure 3, right). For those locations with valid observations, the model reproduces notably well the SO_2 levels. Power plant plumes are included in the HERMES estimations and the plumes dispersion is well characterized by the CALIOPE system (Figure 3, left).
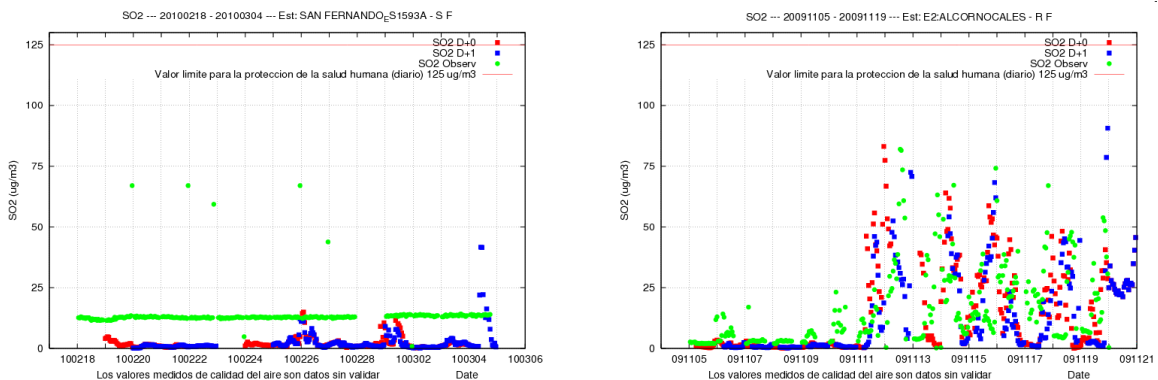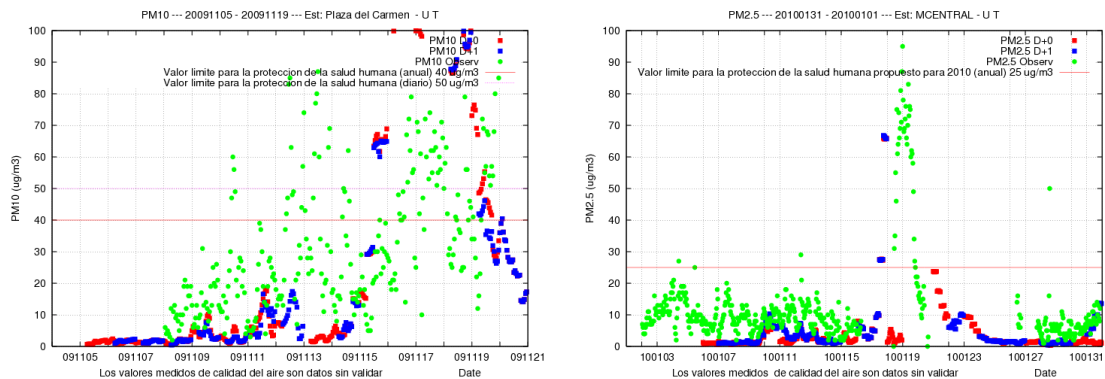

Figure 3. (Left) Hourly SO_2 concentration as predicted by the CALIOPE system for D+0 and D+1 against observed SO_2 from a suburban background station showing a flat profile (SO_2 levels below the detection limits) (Right) Hourly SO_2 concentration as predicted by the CALIOPE system for D+0 and D+1 against observed SO_2 from a rural background station, located near a coal power plant

Particulate matter levels in Spanish urban areas are frequently over the health protection limits established by the EU directives (50 µg m^{-3} – 24 hr mean). Moreover, frequent Saharan Dust intrusions affect the Iberian Peninsula, raising the PM_{10} and $PM_{2.5}$ levels. CALIOPE tends to underestimate PM_{10} levels (it should take in consideration that the observations are raw data of automatic measures systems without using any correction factors), except when a natural dust outbreak occurs (Figure 4, left). This is attributed to the high relative contribution of this natural source and to the good predictability skills of the BSC-DREAM8b model (Jiménez-Guerrero et al., 2008b). The low PM_{10} levels predicted in other cases are attributed to the lack of some emission sources, such as wind blown dust, and to uncertainties on the chemical mechanism leading to secondary particles formation. The observations of $PM_{2.5}$ are scarce and no conclusions can be derived from their analysis, although the behaviour of $PM_{2.5}$ predictions is expected to be similar to that of PM_{10} (e.g. Figure 4, left) .

Figure 4. (Right) Hourly PM_{10} concentration as predicted by the CALIOPE system for D+0 and D+1 against observed PM_{10} from an urban traffic station; (Left) Hourly $PM_{2.5}$ concentration as predicted by the CALIOPE system for D+0 and D+1 against observed $PM_{2.5}$ from an urban traffic station.

The predictions for the first and second day of simulation were treated separately in order to assess the degradation of the model outputs with time. No significant differences between D+0 and D+ 1 prediction were found.

The comparison of the vertical O_3 profiles with observations suggests good predictability skills in the lowest layers. Nevertheless, deviations between model and observations arise with height (Figure 5). The relatively low vertical resolution of the CMAQ model, 15 σ-vertical layers up to 50 hPa, can be one of the reasons of the origin of these discrepancies. The thickness of the σ-layers increases with altitude, the dilution effect being more important. Using a higher vertical resolution could improve these results, but increase the computational time, which is a critical factor in an operational system such as CALIOPE.
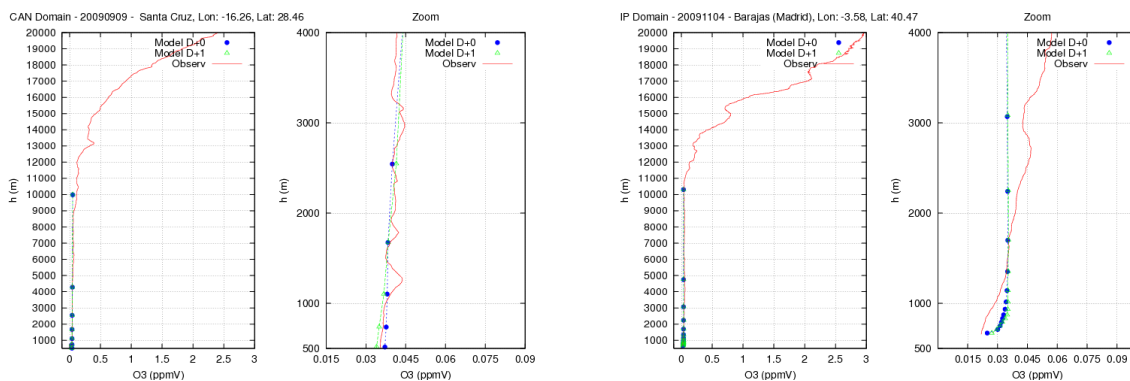

Figure 5. O_3 Vertical profiles comparison for Canarias (left) and Madrid (right)

The EU12 tropospheric column density of NO_2 as provided by the CALIOPE system is compared daily to the AURA OMI product as processed by KNMI. Such a comparison shows that CALIOPE reproduces well the NO_2 patterns over Europe.
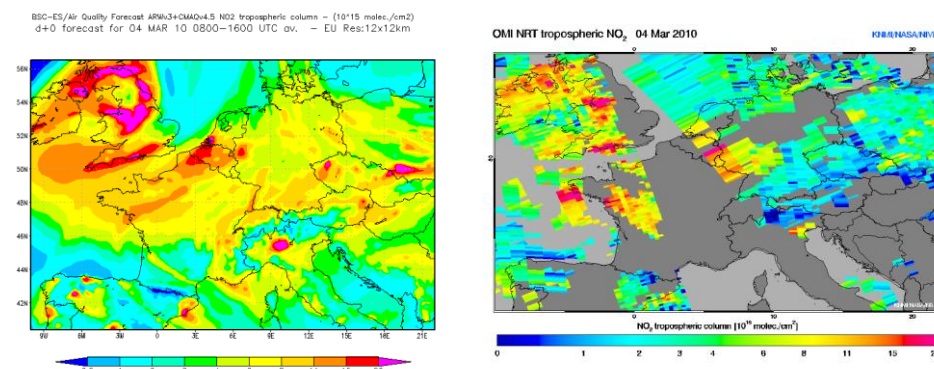

Figure 6. Tropospheric NO_2 column density (10^{15} molec cm^2) as estimated by WRF-ARW/HERMES-EMEP/CMAQ/BSC- DREAM8b in Europe (left) and observed by AURA-OMI satellite (right).

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CONCLUSIONS

The NRT evaluation system shows that CALIOPE performs well when predicting ground level concentrations of gaseous pollutants (NO_2, O_3 and SO_2). The high resolution applied and the specifically developed emission inventory are key factors in this behaviour, providing i.e. a good characterization of NO_2 concentrations in densely populated areas and of SO_2 levels derived from power plants emissions. The dynamics of O_3 are well described, especially in the cases where large NO_x emission sources are present. Some improvements have to be made for rural areas with no influence of urban plumes, to better capture the daily O_3 variation; nevertheless, the background concentration is properly predicted. The mineral dust contribution estimated by BSC-DREAM8b model is a key factor for the improvement in predictions of PM_{10} levels, nevertheless the lack of some sources in the emissions input and the uncertainties in chemical production involve a frequent underestimation of this pollutant. The availability of observations of particulate matter composition and fine fractions ($PM_{2.5}$, PM_1) concentration would be valuable information to improve these predictions. The vertical O_3 profile is well reproduced in the lowest layers, but higher vertical resolution would be needed to capture some vertical structures at height. The model predicts well the patterns of NO_2 vertical column density across Europe, as shown in the qualitative comparison with AURA OMI images.

The CALIOPE NRT evaluation system is still under development, and among the on-going tasks, the quantitative evaluation of the whole 2009, already in progress, deserves mention.

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