Evaluating WRF-BEP/BEM performance: on the way to analyze urban air quality at high resolution using WRF-Chem+BEP/BEM

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Abstract. Air pollution exposure is a major environmental risk to health and has been estimated to be responsible for 7 million premature deaths worldwide every year. This is of special concern in cities, where there are high levels of pollution and high population densities. Not only is there an urgent need for cities to monitor, analyze, predict and inform residents about the air quality, but also to develop tools to help evaluate mitigation strategies to prevent contamination. In this respect, the Weather Research and Forecasting model coupled with chemistry (WRF-Chem) is useful in providing simulations of meteorological conditions but also of the concentrations of polluting species. When combined with the multi-layer urban scheme Building Effect Parameterization (BEP) coupled with the Building Energy Model (BEM), we are furthermore able to include urban morphology and urban canopy effects into the atmosphere that affect the chemistry and transport of the gases. However, using WRF-Chem+BEP/BEM is computationally very expensive especially at very high urban resolutions below 5km. It is thus indispensable to properly analyze the performance of these models in terms of execution time and quality to be useful for both operational and reanalysis purposes. This work represents the first step towards this overall objective which is to determine the performance (in terms of computational time and quality of results) and the scalability of WRF-BEP/BEM. To do so, we use the case study of Metropolitan Area of Barcelona and analyze a 24-hour period (March 2015) under two with different Urban schemes (Bulk and BEP/BEM). We analyze the execution time by running the two experiments in its serial configuration and in their parallel configurations using 2, 4, 8, 16, 32 and 64 cores. And the quality of the results by comparing to observed data from four meteorological stations in Barcelona.

Keywords: WRF-BEP/BEM \cdot WRF-Chem \cdot Scalability \cdot Air Quality \cdot Urban scale

1 Introduction

Understanding urban atmosphere behavior is fundamental to know how air pollution exposure affects citizens. Air pollution exposure is a significant environmental risk to health in highly populated areas and is responsible for an estimated 7 million people deaths every year worldwide ([17]; [6]), which is 3.5 times more deaths than for COVID-19 in 2020 ([3]). Countries can reduce serious diseases by reducing air pollution levels in their major cities and making them more sustainable. Simulation and analysis of the urban atmosphere and air pollution in our cities can help the public to be more informed and urban planners to make better decisions. However, urban air quality models are complex, mainly due to the diversity of spatio-temporal scales on which the phenomena occur. In particular, two essential scales are involved ([8]):

- 1. An 'urban' scale of a few tens of kilometers (city size), where the primary pollutants are emitted;
- 2. A 'meso' scale of a few hundreds of kilometers, where the secondary pollutants are formed and dispersed.

The dispersion of pollutants depends on the structure of the urban boundary layer and its interactions with the rural boundary layer and the synoptic flow. Being a nonlinear system, it is common to use numerical models to study air pollution problems. In order to compute the mean and turbulent transport and the chemical transformations of pollutants, several meteorological variables are needed (wind, turbulent coefficients, temperature, pressure, humidity), which can be interpolated from measurements or computed with mesoscale circulation models. These models must, indeed, ideally be able to represent the two main scales (the 'urban' and the 'meso') involved. Since the horizontal dimensions of the domain are on the order of the mesoscale (100 km), to keep the number of grid points compatible with the CPU time cost, the horizontal grid resolution of such (mesoscale) models ranges, in general, between several hundreds of metres and a few kilometres. This means that it is not possible to resolve the city structure in detail (buildings or blocks), but that the effects of the urban surfaces must be parameterised. Another obstacle to a complete resolution of the city structure is given by the difficulty to provide the necessary input data ([8]).

For that purpose, as a first step, we use the Weather Research and Forecasting (WRF) model with the incorporation of the urban canopy model Building Energy Parameterization and Building Energy Model (BEP/BEM) to take into account the urban morphology ([12],[11]). After that, we will use WRF coupled with chemistry (WRF-Chem; [4]), which adds calculations with chemical substances to the weather simulations, including additional emission files and chemical traces. However, WRF-Chem coupled with BEP/BEM is computationally very expensive, either for reanalysis or operational purposes and especially at very high urban resolutions, so that it makes indispensable understand WRF-Chem + BEM/BEM computational behaviour helping its users and developers to better exploit computational resources using computational strategies in High

Performance Computing (HPC) platforms. This work represents the first step towards this global objective. Concretely, this paper presents the WRF-BEP/BEM scalability. The quality of the results provided has been analyzed for a study case of March 11th, 2015, in Barcelona's urban area (Spain).

This paper is organised as follows. Section 2 describes the Weather Research and Forecasting (WRF) model and the Building Effect Parameterization coupled to the Building Energy Model (BEP/BEM) and describes the experimental study case. Section 3 presents the model scalability and it also includes an analysis of the quality results by comparing the model outputs to the observations. Finally, section 4 summarizes the main conclusions and future work.

2 Data and methods

2.1 Modelling system

Weather Research and Forecasting Model (WRF): The Weather Research and Forecasting (WRFV4) model is an atmospheric modeling system designed for both research and numerical weather prediction ([14]). The Advanced Research WRF (ARW) dynamics solver integrates the compressible, non-hydrostatic Euler equations with several physics schemes and dynamics options designed to phenomena at regional scale ([14]). The WRF-ARW model was developed by NCAR among other organisations and is designed to be an efficient massively-parallel code to be able to take advantage of advanced highperformance computing systems ([13]).

Building Effect Parameterization coupled to the Building Energy

Model (BEP/BEM): As more than half of the world's population lives in urban areas and this proportion is expected to grow up to 64-69% by 2050 ([18]), there is a growing interest in simulating the urban atmosphere and its complex dynamics. For that reason, with the aim of reproducing the effects of the urban canopy on the urban boundary layer (UBL) dynamics ([12]), new features has been included in the main WRF parameterization ([1]; [9]). The level of detail and the degree of complexity of these urban parameterizations depends on the number and nature of the processes described and their integration with the primitive equations of the mesoscale model.

The bulk scheme is the simplest approach, included in the Noah Land Surface Model, which modifies several parameters such as roughness length, albedo, volumetric heat capacity and soil thermal conductivity to better represent the reduced wind speed and increased heat storage capacity of urban areas. This scheme estimates heat and momentum fluxes based on the Monin-Obukhov Similarity Theory (MOST) and does not take into account the heterogeneity within the city, i.e., these values apply to all urban areas, regardless of their urban structure ([9], [10]). Urban canopy schemes were developed and included in WRF as physics options. These more advanced urban schemes were explicitly designed to represent city morphology (e.g., building and street canyon geometry) and

surface characteristics (e.g., albedo, heat capacity, emissivity, urban/vegetation fraction). The currently available urban canopy schemes are:

- Single Layer Urban Canopy Model (SLUCM [7]);
- Building Effect Parameterization (BEP, [8]): a multi-layer layer scheme;
- BEP coupled to the Building Energy Model (BEP/BEM, [8], [12]): the second generation of BEP considers energy consumption in buildings (heating/cooling) for a more accurate effect on urban heat budget.

BEP parameterizes a 3D urban morphology in a multi-layer model grid, being capable of estimating the heat fluxes from roofs, ground, and walls, individually ([8]) and computing the impact of buildings on the airflow and turbulence (term included in the conservation equation for the Turbulent Kinetic Energy – TKE), as well as the source/sinks of heat by solving the energy budget for each surface ([9]; [8]). Unlike BEP that keeps the indoor temperature constant, BEP/BEM calculates the anthropogenic heat generated by air conditioning systems and the heat exchanges between the building's interior and the outer atmosphere ([10], [12]). In this work, BULK and BEP/BEM options are evaluated to study the computational performance of such schemes (see Table 1) in the Barcelona urban region.

WRF schemes	Bulk	BEP/BEM	
Urban scheme	Included in the Noah (LSM) BEP/BEM		
	Land Surface Model		
Land Surface Model	Noah LSM		
PBL scheme	Bougeault-Lacarrère PBL (BouLac), designed to use with urba		
	schemes		
Microphysics	WRF Single Moment 6-class scheme		
Long- and short-	Rapid Radiative Transfer Model for G	eneral circulation models	
wave radiation	(RRTMG) scheme		

Table 1. Parameterizations used for each experiment (same as in [10]

Atmospheric Chemistry using WRF-Chem: WRF-Chem is a full online atmospheric chemistry model with many options and some interactions with physics aerosols affecting radiation and microphysics. Typically it requires emission source maps as additional inputs ([14]; [4]). Although the complete study will include this feature, in this work, as it was previously mentioned, we do not consider the Chem module.

2.2 Experimental Study Case

The study case selected was the day March 11, 2015 which corresponds to a day within a period of high temperatures in Catalonia (North-East of Spain).

From the 1st to the 13th of March 2015 the meteorological situation in Catalonia was marked by a strong anticyclone that stabilised the atmosphere and caused a significant increase in temperature. It is worth mentioning that in certain stations with more than 20 years of data, recorded the maximum temperature value for all recorded series for the first half of March ([15]). Due to the anticyclone and the high pressure situation, urban air pollution also increased in Barcelona making this a good period to study both the urban heat (WRF-BEP/BEM) as well as urban pollution and atmospheric chemistry (WRF-Chem). This work focuses on urban heat and scaling simulations of WRF and WRF-BEP/BEM. To simulate the study region, two two-way nested domains were defined. The parent domain (Iberian Peninsula) with a horizontal resolution of 9 km×9 km (WE: 1350 km, NS: 1305 km), followed by a finer domain comprehending the Catalonia region at 3 km ×3 km horizontal resolution (WE: 354 km; NS: 354 km) (Figure 1). Vertically, both domains are described by 57 layers (model top pressure: 0.1 hPa).



Fig. 1. Simulation domain configuration. D01: Iberian Peninsule (IP), D02: Catalonia (CAT) with 9 km x 9 km and 3 x 3 km horizontal resolution, respectively.

As initial and boundary meteorological conditions to the parent domain we use ERA5 reanalysis ([5], [16]), from the European Center for Medium-Range

Weather Forecasts (ECMWF), which provides hourly data and a good resolution of 0.25 degree (31 km).

3 Results

3.1 Quality Results

The observational data used to evaluate the WRF output was provided by the Meteorological Service of Catalonia (SMC). We compared data from four stations located in the Metropolitan Area of Barcelona (see Table 2).

Station	Measurement	Altitude	Latitude	Longitude
acronym		above ground (m)		
Badalona	T, RH	50	41.452	2.248
Raval	T, RH, W	40	41.384	2.168
Zuni	T, RH, W	10	41.379	2.105
ObsFabra	T, RH, W	411	41.418	2.124

 Table 2. Meteorological Stations

Temperature (T): In Figure 2, we can observe the temperature daily profile comparison from the stations of Badalona, Raval, Zona Universitaria (ZUni), and Observatori Fabra (ObsFabra). Figure 2(a) shows the observed temperature against the obtained temperature from bulk and BEP/BEM simulations. From 00 to 03h the simulations estimate an increase in the temperature while we observe a reduction of the observational value. During this period time, both implementations underestimate the temperature. From 6 o'clock, we can see that both models estimate an increase of the temperature until reaching a peak at noon. The simulations and observations follow a similar temperature variation trend from this hour on. Figure 2(b) shows that BEP/BEM tends to overestimate the temperature value more than BULK except between 9 and 18 o'clock. Neither of the two models accurately describes the observations since they both underestimate the T by about two degrees at midday. Figure 2(c) shows that the two schemes give higher temperature values during the whole day. The trend of the simulated temperature variation is close to the observed one. In Figure 2(d), the observed temperature is approximately constant from 00 to 09h, while the two schemes predict an increase in temperature from 00 till to 12h. The two simulations describe correctly the evolution of the temperature. From 18h, the simulations underestimate again, estimating a decrease in temperature while the observations indicate that the temperature remained constant.



Fig. 2. Temperature. Bulk (blue line) and BEP+BEM schemes (orange line) comparison with meteorological observation (black line)

Relative Humidity (RH): In Figure 3(a), we can see both simulations tend to underestimate the RH except from 00 to 02h that underestimate it. During these hours of the day RH is high in the four stations, after compare with ERA5 global model it seems that this high RH's come from initial conditions. Figure 3(b) shows that the RH is underestimated from 03 to 09h and from 17 to 00h, while in central hours, between 9 and 17h, the simulation estimates are very close to reality. Moreover, BULK is maintained with a higher temperature all day long. In Figure 3(c) we can see similar case to Raval, but in this case, BEP/BEM estimates higher relative humidity than bulk, being closer to the value of the observations. Figure 3(d) presents that the model estimates the observed relative humidity better at low RH, while in night hours, the simulation estimates and the observations diverge.

Wind Speed (WS) In the Figures 4(a) and 4(b), both simulations describe the wind speed trend, but BEPBEM fits better to reality in this simulation. In



Fig. 3. Relative Humidity. Bulk (blue line) and BEP/BEM schemes (orange line) comparison with meteorological observation (black line)

4(b) BEP/BEM fits again very well and better than bulk, which overestimates in 1.5m/s the wind speed value. Figures 4(c) and 4(d) show that BEP/BEM underestimates the wind speed. Instead, Bulk at (4(c)) overestimates it from 00 to 9 o'clock, in central hours of the day it follows a similar tendency and from 20 o'clock it overestimates the wind speed. In 4(d) the tendency at the end of the day, from 18h, tends slightly to observation values.

For more results in this region using WRF-BEP/BEM see the study carry out by Ribeiro et al. (2021) [10].

3.2 Scalability Results

The computing platform used for these experiments using distributed memory is a multi-core system composed of 2 sockets with AMD EPYC 7551 32-Core Processors each and a total of 128 CPUs (64 cores and 128 threads). In order to analyse the parallelization and the scalability of WRF-BEP/BEM, we have



Fig. 4. Wind Speed. Bulk (blue line) and BEP/BEM schemes (orange line) comparison with meteorological observation (black line)

executed the two experiments in its serial configuration and in their parallel configurations using 2, 4, 8, 16, 32 and 64 cores.

WRF-BEP/BEM has been parallelized using MPI. The MPI parallelization is done through patches; that is, the domain is divided into a fixed number of parts according to the number of cores available for a given simulation. These p ince each patch needs information from its neighbors' patches to run the model, each patch includes extra points (called halo) to incorporate those points from the four borders that are required to execute on one iteration of the model. After finishing each iteration, the patches must exchange the results from the points in the halo. Therefore, a synchronization barrier is required. This scheme implies that all MPI processes proceed in a synchronized fashion what can imply non-depreciable communication time if the patch size is not well evaluated ([2]).

Figure 5 shows execution times for each experiment. As we can see, BEP/BEM scheme needs higher execution times, especially for his serial configuration, in the parallel configuration there are less difference in time execution



Fig. 5. WRF-BEP/BEM Execution time when running a 24 hours simulation

between both schemes but is still higher in BEP/BEM. At 32 cores and above, we can see that allocating more resources does not result in a reduction of execution time proportional to the resources invested. From 32 cores to 64 cores only have a time execution improvement of 10 minutes with BEP/BEM and 3 minutes with Bulk.

Figure 6 also shows that Bulk scales well up to 32 cores where the curve starts to flatten, and we do not have the performance improvement we would expect at 64 cores, getting a speedup of x20. In WRF-BEP/BEM, although the curve also begins to flatten, we are getting a speedup of x39 with 64 cores.

4 Conclusions and Future Steps

Urban air quality models are complex, mainly due to the diversity of spatiotemporal scales on which these phenomena occur. To evaluate the air quality in urban zones, the combination of both WRF-Chem model including BEP/BEM. However, these coupled models are computationally very expensive, especially at very high urban resolutions and for these reason we start evaluating the WRF-BEP/BEM performance.

This work represents the first step towards this global objective. Concretely, this paper has presented the WRF-BEP/BEM scalability. The quality of the results provided has been analyzed for a study case of March 11th, 2015, in Barcelona's urban area (Spain).

The analysis performed of both implementations, Bulk and BEP/BEM, describes the evolution of temperature and humidity similarly. They have some

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Fig. 6. WRF and WRF-BEP/BEM Speed Up when executing a 24 hours simulation.

differences in wind speed, more accurate estimation of BEP/BEM in this simulation. However, these are preliminary results, and we need to simulate more days and analyze more stations to reach better quality results.

Regarding the scalability analysis, the main problem we face is that BEP/BEM is computationally more expensive than Bulk. Moreover, in this work, we only considered two domains with a 3km resolution, and BEP/BEM substantially increases the resource requirements by adding the third domain with a resolution of 1 km. For this reason, the execution time spent by BEP/BEM slightly differs from the time invested in Bulk. BEP/BEM configuration scales better than Bulk, which reaches its maximum performance when using 32 cores. At the same time, BEP/BEM could still reduce the execution time by increasing the number of cores.

Future steps will be oriented to complete the Bulk and BEP/BEM's scalability study introducing a third domain of 1 km-resolution. After that, we will continue our study introducing WRF-Chem and WRF-Chem+BEP/BEM configuration and studying their scalabilities and computational performance, always taking into account the simulations' quality results. Once we have the complete WRF-Chem+BEP/BEM scalability study, we will analyze and evaluate WRF-Chem+BEP/BEM bottlenecks and apply computational strategies to run WRF-Chem+BEP/BEM at urban resolutions while using moderated execution times.

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