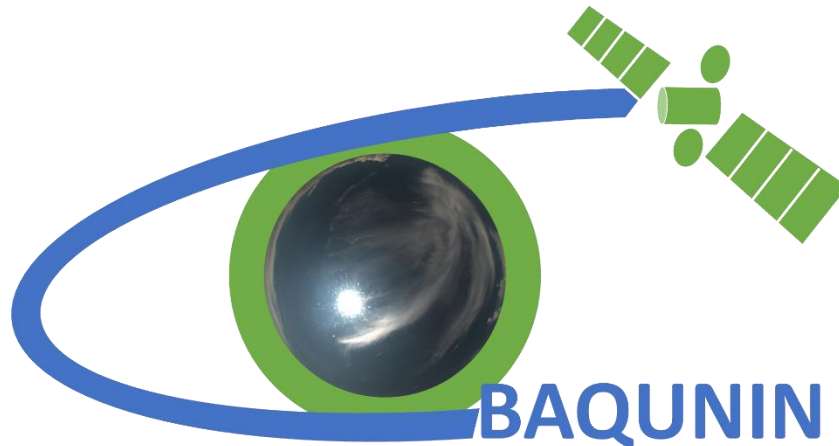


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WRF configuration and trajectory calculations

Abstract This is the delivery D-3.6 as part of WP-3000.

Author Enrico Cadau, Andrea Murgia,
on behalf of BAQUNIN Team

Approval Angelika Dehn
ESA/ESRIN Technical Officer

Distribution ESA/ESRIN EOP-GMQ
BAQUNIN Leadership Team

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Serco Italia SpA

Sede Operativa: Via Sciadonna, 24-26 - Frascati (Roma)

Tel: +39 06 98354400 Fax:

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1. INTRODUCTION

This document represents the deliverable D-3.6 as part of the WP 3100. It describes the meteorological model WRF configuration parameters adopted in the BAQUNIN project and details the trajectory calculations module implemented.

1.1 Reference Documents

[RD.1] WRF Version 3 Modelling System User Guide - 2016

2. WRF

2.1 Introduction

Meteorology plays a crucial role in air quality monitoring (AQM). In this document we describe a most recent version of the meteorological model called Weather Research and Forecasting (WRF) model and its importance in air quality applications in the framework of Baquinin project. The performance of WRF depends upon the intended application and parameterization scheme of physics options. WRF model is also applied to investigate the simulation results with various land surface models (LSMs) and Planetary Boundary Layer (PBL) parameterizations and various set of microphysics options. It predicts various meteorological spatial parameters like mixing layer height, air temperature, humidity, rain fall, cloud cover and wind. The WRF output results are used in the Baquinin project to predict atmosphere's conditions and to provide trajectories of pollutant components.

Meteorological processes include horizontal and vertical transport, turbulent mixing and convection of pollutants. The main requirement of meteorological data for air quality modelling can be accomplished by either onsite monitoring or meteorological modelling.

Meteorological models calculate three-dimensional gridded meteorology using mathematical equations to simulate atmospheric processes like the variation in temperature and winds over time. The main purpose of the meteorological model is to forecast and simulate the weather parameters using current observed meteorological parameters.

These models forecast meteorological parameters by solving equations (e.g. Navier-Stokes equations) of mechanics for a compressible fluid which are derived from the three fundamental physical laws governing all geophysical processes i.e., conservation of mass (for wind and moisture), momentum (Newton's laws of motion), and thermal energy (the first law of thermodynamics). The equations arising out of these three laws estimate the weather parameters from physical phenomena and strongly interact with each other. A research and development group on air quality has developed methods of meteorological forecast for predicting the atmospheric dispersion, decay and decomposition of radioactive material.

The Weather Research and Forecasting (WRF-ARW ([Skamarock et al. 2008](#))) Model developed at NCAR in the United States is a non-hydrostatic, incompressible numerical weather prediction (NWP) model that has been used in various research studies. The WRF is a state of the art mesoscale numerical weather prediction system designed to apply to both meteorological research and numerical weather prediction needs (Henmi et al., 2005).

The model has the ability to simulate and forecast, followed by producing a meteorological profile that reflects either real data or ideal data of the atmospheric condition downscaling initialisation global model data. WRF has increasingly been used in both military and private meteorological fields and has also been adopted by the NOAA's National Weather Service (NCAR, 2012).

Over recent decades, many different parameterizations have been proposed for this model, especially for the PBL (Planetary Boundary Layer). PBL parameterizations are responsible for vertical subgrid-scale fluxes, allowing eddy transports through the entire atmospheric column. Wind distribution is affected by factors such as PBL height, wind shear, and entrainment of free atmospheric air into the PBL, which determines momentum, heat, and moisture exchanges at the top of the layer ([Arya 2001](#)).

2.2 Model Structure

WRF Modeling System Flow Chart

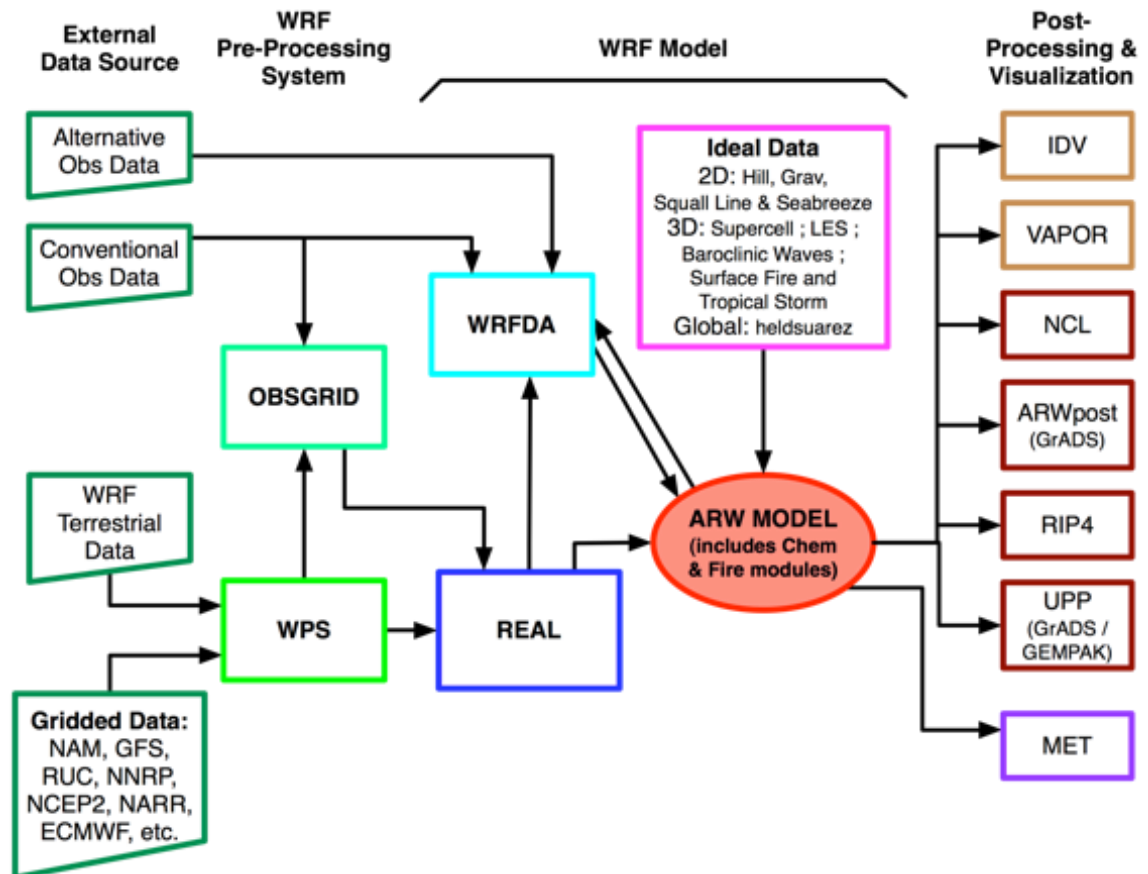


Figure 1 - General WRF flow chart

As shown in the diagram of Figure 1, the WRF Modeling System consists of these major programs:

- The WRF Preprocessing System (WPS).
- WRF-DA (Data Assimilation): not used in this contest.
- ARW solver.
- Post-processing & Visualization tools.

2.2.1 WPS

The WRF Preprocessing System (WPS) is a set of three programs whose collective role is to prepare input to the real program for real-data simulations.

This set is used primarily for real-data simulations. Its functions include 1) defining simulation domains; 2) interpolating terrestrial data (such as terrain, landuse, and soil types) to the simulation domain; and 3) degribbing and interpolating meteorological data from another model to this simulation domain. Its main features include:

- GRIB 1/2 meteorological data from various centers around the world
- USGS 24 category and MODIS 20 category land datasets

- Map projections for 1) polar stereographic, 2) Lambert-Conformal, 3) Mercator and 4) latitude-longitude.
- Nesting
- User-interfaces to input other static data as well as met data.

Each of the programs performs one stage of the preparation: geogrid defines model domains and interpolates static geographical data to the grids; ungrib extracts meteorological fields from GRIB formatted files; and metgrid horizontally interpolates the meteorological fields extracted by ungrib to the model grids defined by geogrid. The work of vertically interpolating meteorological fields to WRF eta levels is performed within the real program.

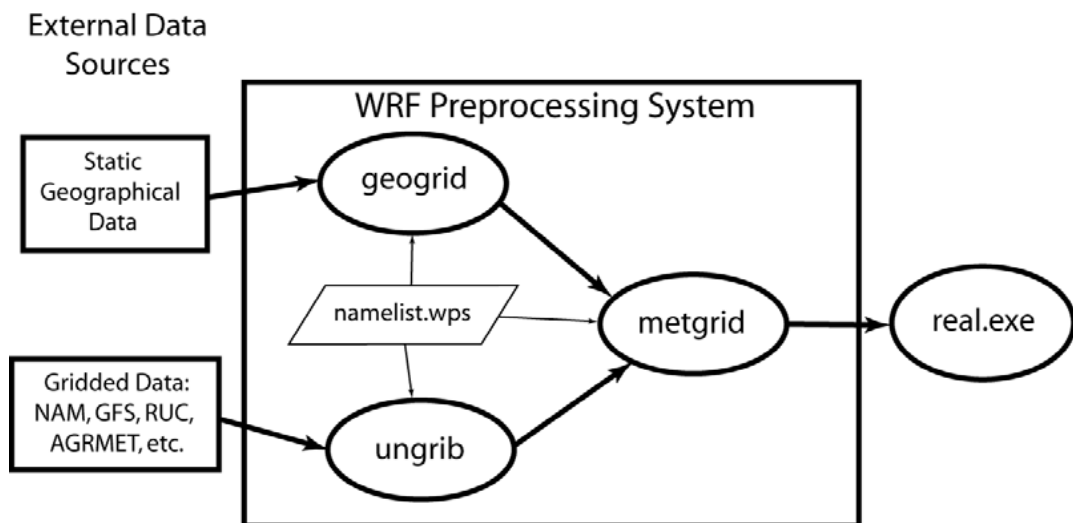


Figure 2 – Main WRF components and interfaces

The data flow between the programs of the WPS is shown in the figure above. Each of the WPS programs reads parameters from a common namelist file, as shown in the figure.

This namelist file has separate namelist records for each of the programs and a shared namelist record, which defines parameters that are used by more than one WPS program.

Not shown in the figure are additional table files that are used by each individual executable.

These tables provide additional control over the programs' operations, though they generally do not need to be changed by the user. The GEOGRID.TBL, METGRID.TBL, and Vtable files are explained in [RD.1], though for now, the user need not be concerned with them.

2.2.2 WRF-ARW

This is the key component of the modelling system, which is composed of several initialization programs for idealized, and real-data simulations, and the numerical integration program. The key features of the WRF model include:

- Fully compressible non-hydrostatic equations with hydrostatic option
- Regional and global applications
- Complete Coriolis and curvature terms
- Two-way nesting with multiple nests and nest levels

- Concurrent one-way nesting with multiple nests and nest levels
- Offline one-way nesting with vertical nesting
- Moving nests (prescribed moves and vortex tracking)
- Mass-based terrain-following coordinate
- Vertical grid-spacing can vary with height
- Map-scale factors for these projections:
 - polar stereographic (conformal)
 - Lambert-conformal
 - Mercator (conformal)
 - Latitude and longitude, which can be rotated
- Arakawa C-grid staggering
- Runge-Kutta 2nd and 3rd order time integration options
- Scalar-conserving flux form for prognostic variables
- 2nd to 6th order advection options (horizontal and vertical)
- Monotonic transport and positive-definite advection option for moisture, scalar, tracer, and TKE
- Time-split small step for acoustic and gravity-wave modes:
 - small step horizontally explicit, vertically implicit
 - divergence damping option and vertical time off-centering
 - external-mode filtering option
- Upper boundary absorption and Rayleigh damping
- Lateral boundary conditions
 - idealized cases: periodic, symmetric, and open radiative
 - real cases: specified with relaxation zone
- Full physics options for land-surface, planetary boundary layer, atmospheric and surface radiation, microphysics and cumulus convection
- A single column ocean mixed layer model
- Grid analysis nudging using separate upper-air and surface data, and observation nudging
- Spectral nudging
- Digital filter initialization
- Adaptive time stepping
- Gravity wave drag

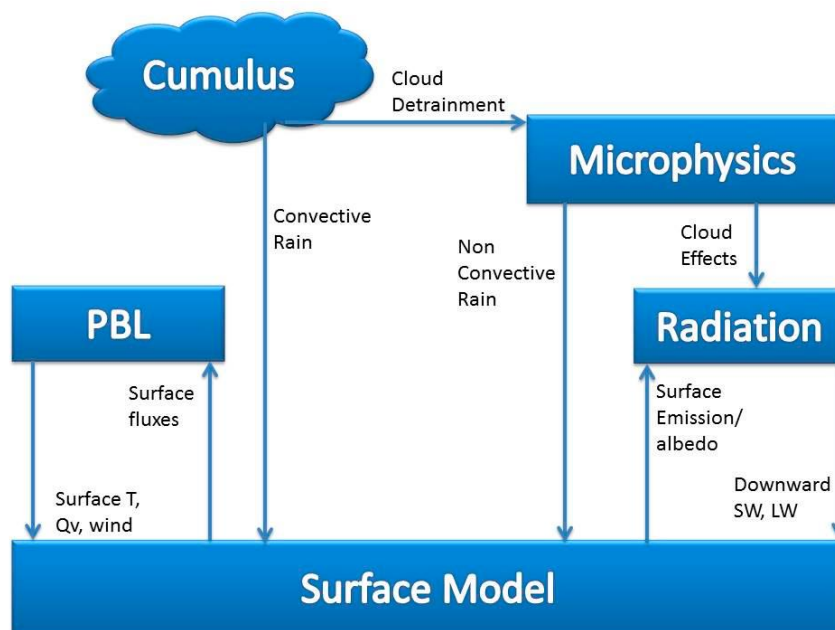


Figure 3 – High Level interaction schema of all the parameterisations

Figure 3 shows the interaction schema of all the various parametrization with the Surface Model.

2.2.3 Governing Equations

The ARW dynamics solver integrates the compressible, nonhydrostatic Euler equations. The equations are cast in flux form using variables that have conservation properties, following the philosophy of Ooyama (1990). This set of equations is formulated using hydrostatic pressure as an independent variable (Laprise, 1992). The vertical coordinate is terrain following, using a hybrid $\sigma - p$ formulation.

The ARW equations are formulated using a terrain-following hydrostatic pressure vertical coordinate denoted by η and defined as: $\eta = (p_h - p_{ht})/\mu$ where $\mu = p_{hs} - p_{ht}$. p_h is the hydrostatic component of the pressure, and p_{hs} and p_{ht} refer to values along the surface and top boundaries, respectively (cf. Figure 4).

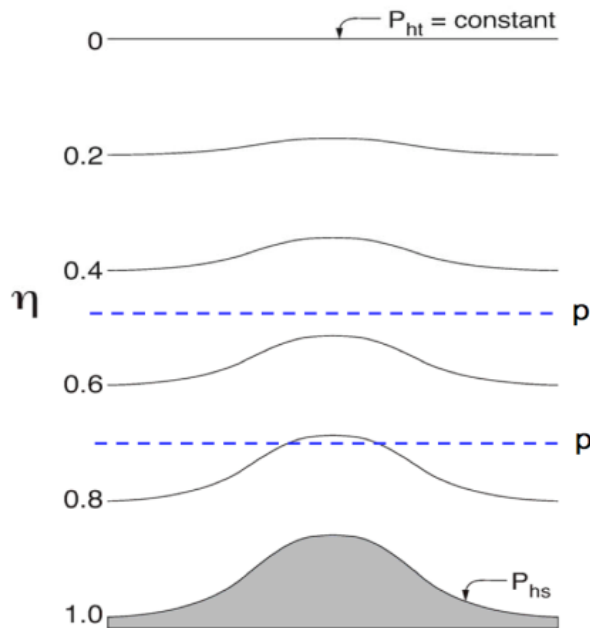


Figure 4 - In WRF Model, vertical coordinate is normalized hydrostatic pressure

η varies from a value of 1 at the surface to 0 at the upper boundary of the model domain. This vertical coordinate is also called a mass vertical coordinate. Also appearing in the governing equations of the model are the non-conserved variables:

- $\phi = g_z$ (the geopotential);
- p (pressure);
- $\alpha = 1/\rho$ (the inverse density).

For simplicity of interpretation we will view the flow in Cartesian coordinates and neglect the Coriolis effect. With these restrictions, the WRF model can be configured to solve the following equations:

Equation of State

$$p = \rho R_d T;$$

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} = 0;$$

Conservation of Momentum

$$\frac{\partial U}{\partial t} + c_p \Theta \frac{\partial \pi}{\partial x} = -\frac{\partial Uu}{\partial x} - \frac{\partial Vu}{\partial y} - \frac{\partial Wu}{\partial z} + F_x,$$

$$\frac{\partial V}{\partial t} + c_p \Theta \frac{\partial \pi}{\partial y} = -\frac{\partial Uv}{\partial x} - \frac{\partial Vv}{\partial y} - \frac{\partial Wv}{\partial z} + F_y,$$

and

$$\frac{\partial W}{\partial t} + c_p \Theta \frac{\partial \pi}{\partial z} + g\rho = -\frac{\partial Uw}{\partial x} - \frac{\partial Vw}{\partial y} - \frac{\partial Ww}{\partial z} + F_z;$$

Conservation of Energy

$$\frac{\partial \Theta}{\partial t} + \frac{\partial U\theta}{\partial x} + \frac{\partial V\theta}{\partial y} + \frac{\partial W\theta}{\partial z} = \rho Q.$$

and

$$U = \rho u, \quad V = \rho v, \quad W = \rho w, \quad \Theta = \rho \theta,$$

where (v, w) are the velocity components in the (x, y, z) directions, θ is the potential temperature, and ρ is the air density. The other variables appearing above are the absolute temperature T and the Exner function,

$$\pi = (p / p_0)^{(R_d/c_p)},$$

where p is the pressure and $p_0 = 1000$ hPa is a reference value. The specific heat at constant pressure for dry air is given by $c_p = 1004.5$ J K⁻¹ kg⁻¹, and $R_d = (2/7)c_p$ is the gas constant for dry air; x, y, and F_x , F_y , and F_z are friction terms.

The RK3 (Runge-Kutta) scheme, described in Wicker and Skamarock (2002), integrates a set of ordinary differential equations using a predictor-corrector formulation. Defining the prognostic variables in the ARW solver as $\Phi = (U, V, W, \Theta, \phi', \mu', Q_m)$ and the model equations as $t = R(\Phi)$, the RK3 integration takes the form of 3 steps to advance a solution $\Phi(t)$ to $\Phi(t+\Delta t)$:

$$\begin{aligned} \Phi^* &= \Phi^t + \frac{\Delta t}{3} R(\Phi^t) \\ \Phi^{**} &= \Phi^t + \frac{\Delta t}{2} R(\Phi^*) \\ \Phi^{t+\Delta t} &= \Phi^t + \Delta t R(\Phi^{**}) \end{aligned}$$

where Δt is the time step for the low-frequency modes (the model time step). Superscripts denote time levels. This scheme is not a true Runge-Kutta scheme per se

because, while it is third-order accurate for linear equations, it is only second-order accurate for non-linear equations.

2.2.4 Post-Processing and Visualization

The post processing consists in the usage of a set of graphic libraries which are in charge of visualising the WRF-ARW output by computing derivative variables such as “dewpoint”, “cumulate rainfall”, etc. In particular NCL, VAPOR and ad-hoc IDL scripts are used in BAQUNIN project.

An example of plot derived from WRF output is shown in Figure 5, where the air temperature in the various height layers.

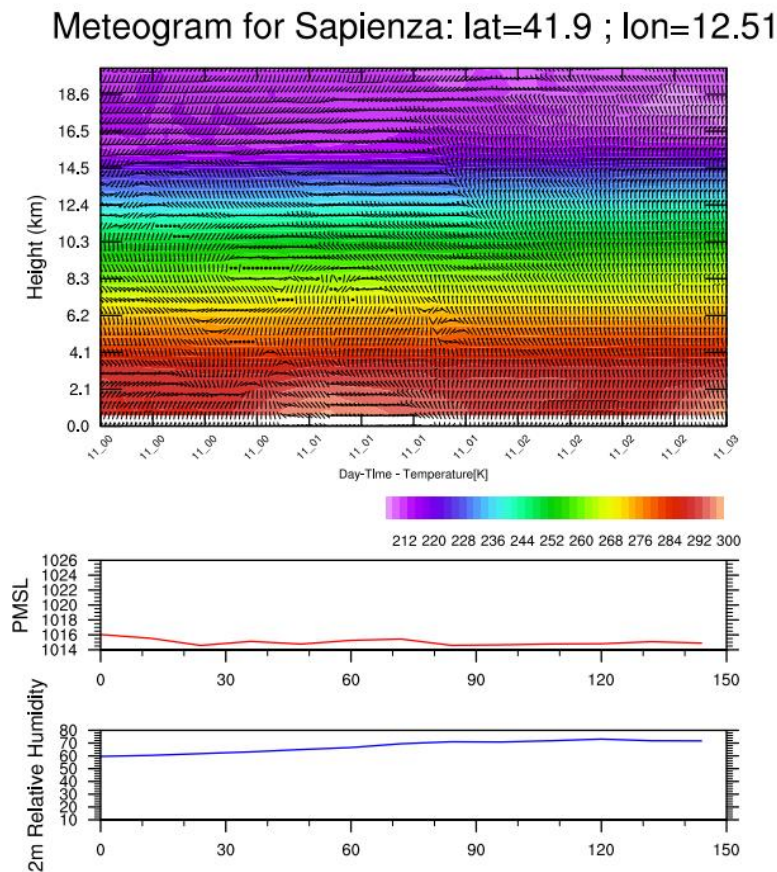


Figure 5 – Example of meteogram computed from WRF output.

2.3 Configuration

This chapter aims at describing the WRF model configuration used in this project. The version of the WRF-ARW core compiled is the 3.9.1 for the real-time processing whereas is 4.0 for the on-demand offline instance. WPS version is already aligned to 4.0 for both. The area covered by the domain is depicted in Figure 6 representing Rome, the Tiber's valley and its suburban areas in central Italy.

The model is configured in the Lambert conformal map projection with the central latitude of 42.2° N and longitude of 12.75° E. It uses three two-way nested domains configuration consisting of a 9 km resolution outer domain, 3 km for the middle and a 1 km on the smaller inner domain with 108 × 108, 106 × 106 and 106 × 106 grid points, respectively (cf. Figure 6). The model configuration for the inner domain uses an ample buffer zone of

five grid points and an exponential transition at the border. Forty vertical levels (from ~30m to 21000m) with a maximum height of 50 hPa are used for all the domains simulations. Such vertical levels are denser on lower atmosphere.

It is initialized using GFS (Global Forecast System) NCEP data version FV3 provided by NOAA at 0.25° of grid resolution with 64 levels in the vertical extending up to 0.2 hPa.

In terms of forecasts the model is configured to predict every day 36 hours of weather conditions in the future with a timestep of 15 min.

WPS Domain Configuration

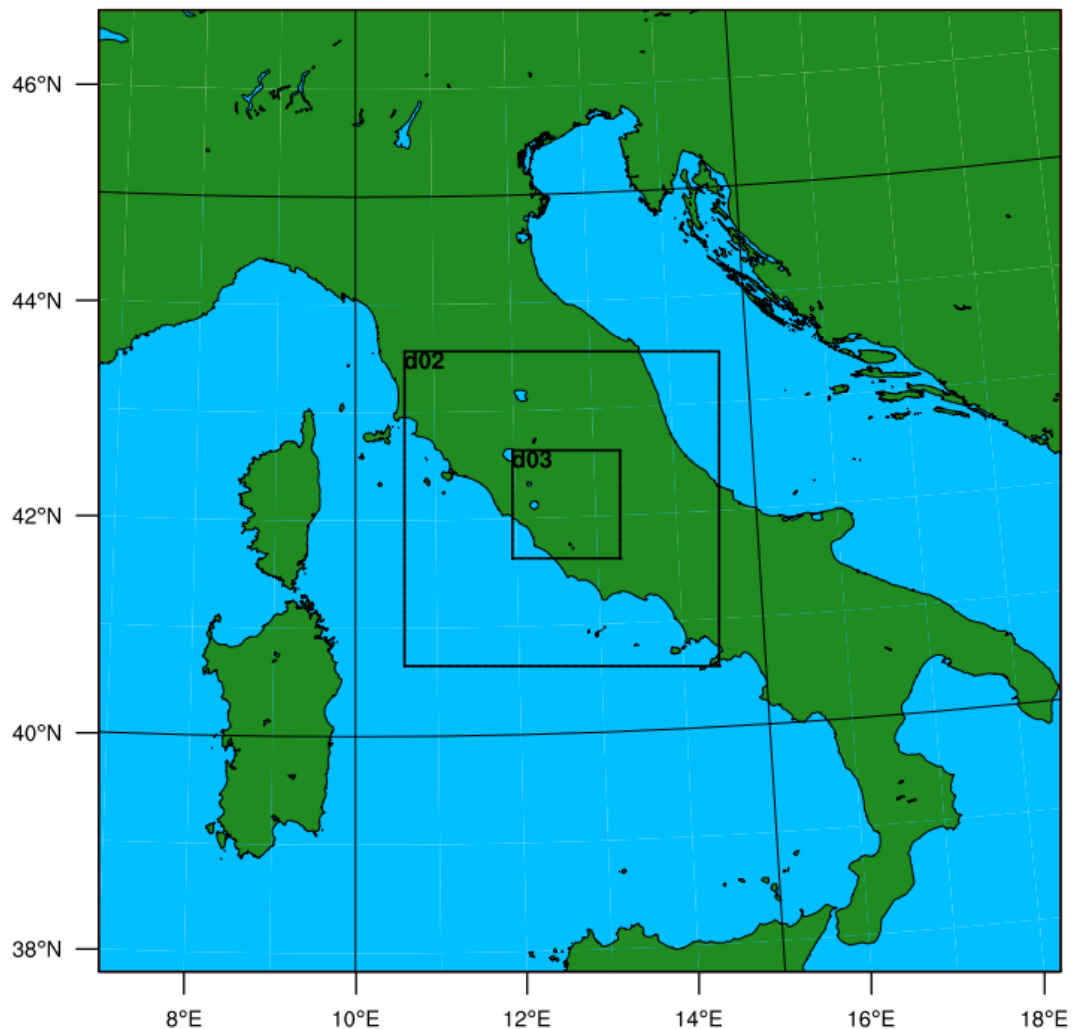


Figure 6 - Geographical coverage of the three domains

2.3.1 WPS parameters

As introduced in chapter 2.2.1 the WPS is in charge of preparing all the input datasets for running the WRF simulations. It comprises in particular the geographical ancillary data such as DEM, Land Use, Land Masks, etc and of course the global model forecasts boundary conditions provided by GFS (Global Forecast System) by the National Centers for Environmental Prediction (NCEP) at NOAA.

GFS data include dozens of atmospheric and land-soil variables from temperatures, winds, and precipitation to soil moisture and atmospheric ozone concentration. A subset covering the Mediterranean Europe is fetched regularly from NCEP server by the BAQUNIN system and then properly handled by the WPS tailored software.

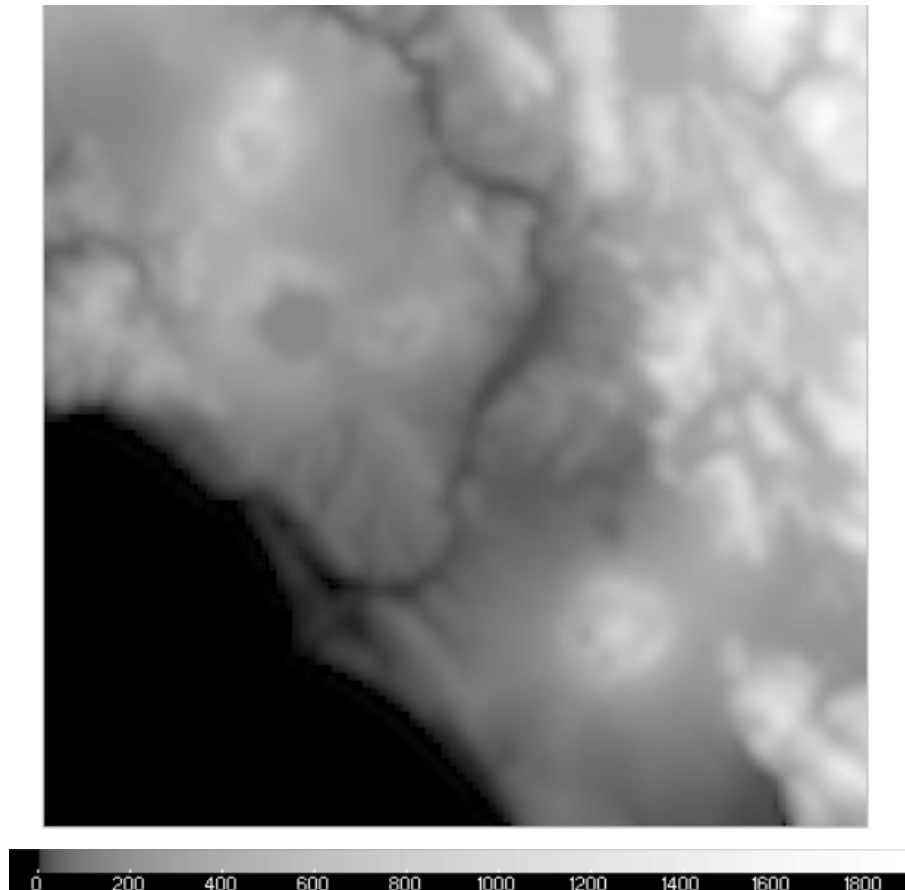


Figure 7 - DEM used for the simulations, the Tiber valley is easily distinguishable.

The output of the WPS is a set of “met” files that include all the boundary conditions at hourly time steps necessary for the ARW core to run.

2.3.2 ARW parameters

The WRF core allows hundreds of possible combinations in terms of parameterisation. We decided to focus on the ones widely tested as more reliable for the boundary layer wind simulation.

2.3.2.1 Namelist.input

This file is the configuration file for all the different kind of parameterisation. It includes the following main features:

```
&physics
  mp_physics          = 8,      8,      8,      8,
  ra_lw_physics       = 1,      1,      1,      1,
  ra_sw_physics       = 1,      1,      1,      1,
```

```

radt                = 10,      3,      1,
SWINT_OPT           = 1,
RA_CALL_OFFSET      = 0,
sf_sfclay_physics   = 1,      1,      1,      1,
IZOTLND            = 1,
sf_surface_physics  = 2,      2,      2,      2,
SF_SURFACE_MOSAIC    = 1,
MOSAIC_CAT          = 1,
SF_LAKE_PHYSICS     = 1,      1,      1,      1,
LAKEDEPTH_DEFAULT   = 50,      50,      70,      70,
bl_pbl_physics      = 1,      1,      1,      1,
YSU_TOPDOWN_PBLMIX  = 1,
SCALAR_PBLMIX       = 1,      1,      1,      1,
bldt               = 0,      0,      0,      0,
cu_physics          = 1,      0,      0,      0,
cudt               = 5,      5,      5,      0,
cu_rad_feedback     = .T.,      .T.,      .T.,
CU_DIAG            = 0,      0,      0,
isfflx             = 1,
ifsnow             = 1,
icloud             = 1,
ISHALLOW          = 1,
surface_input_source = 1,
num_land_cat        = 28,
num_soil_layers     = 4,
sf_urban_physics    = 1,      1,      1,      1,
TOPO_WIND           = 0,      1,      1,      1,
topo_shading        = 1,      1,      1,      1,
slope_rad           = 1,      1,      1,      1,
shadlen            = 25000,
sst_update          = 0,
sst_skin            = 1,
tmn_update          = 0,
lagday             = 0,
usemonalb           = .false.,
rdmaxalb            = .false.,
RDLAI2D            = .false.,
fractional_seaice    = 1,
/

```

In detail for the microphysics option the Thompson graupel scheme with six classes of moisture species plus number concentration for ice as prognostic variables is adopted.

For the long wave radiation option RRTM scheme is used meaning Rapid Radiative Transfer Model. An accurate scheme using look-up tables for efficiency. Accounts for multiple bands, trace gases, and microphysics species.

For the shortwave radiation option Dudhia scheme, simple downward integration allowing for efficient cloud and clear-sky absorption and scattering.

2.4 Infrastructure

All the executables have been compiled using Parallel Intel compiler (both C++ and Fortran) for optimizing the parallelization opportunities of the workstation used. This feature allows to minimize the computation time by using all the cores available in the CPU.

A set of dedicated scripts written in bash and python is in charge of running operationally all the steps of the model (WPS + WRF + Post Processing). In particular they are

devoted to the automatic download of the GFS NCAR input weather data and the generation of the output meteorological maps. The three components of the model run in the same workstation.

The following schema shows the dedicated BAQUNIN WRF processing and archiving infrastructure with the main interfaces. Blue arrows depict http/ftp interfaces, black arrows indicate NFS internal interfaces.

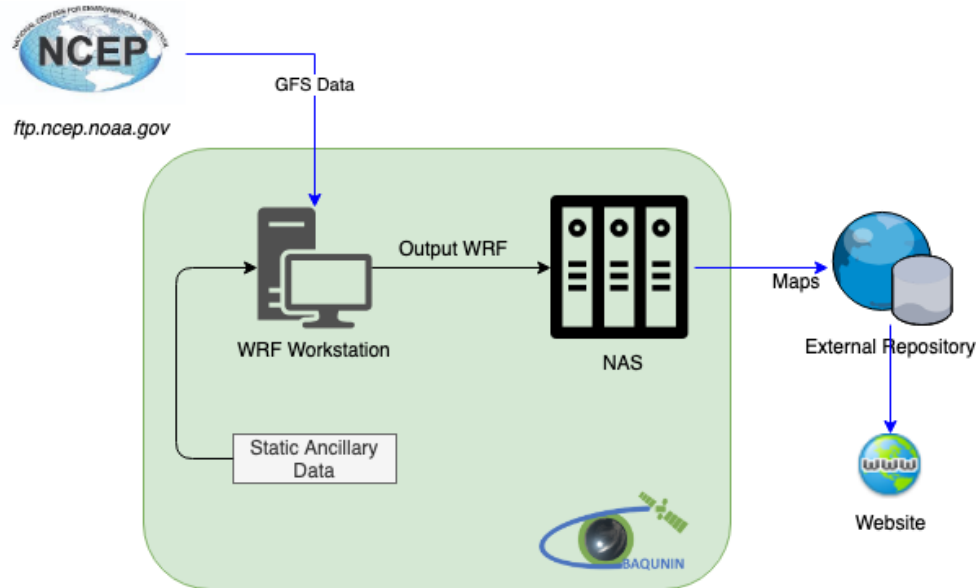


Figure 8 - WRF infrastructure layout within Baqunin.

In terms of data volume, the main ones are specified in the following tables with associated data formats. All the output are regularly stored in a dedicated NAS.

Input Data (Format)	Volume	Frequency
GFS-Meteo (GRIB)	360 MB	Daily
GFS-SST (GRIB)	2 MB	Daily
Geographic Data (ASCII)	5 GB	Static

Table 1 - Input data

Output Data (Format)	Volume	Frequency
WRF (NETCDF)	5 GB	Daily
Maps (PNG/PS/PDF)	50 MB	Daily

Table 2 - Output data

3. TRAJECTORIES CALCULATION

Since version 3.7 WRF introduced a dedicated framework able to create basic tracers as output. The idea is to exploit such a capability to test the dispersion in atmosphere of pollutants and to understand the role of atmospheric stability on the short-term transport of a continuous release passive scalar plume in three different convective boundary layer regimes: highly convective, combined shear and buoyancy and shear dominated. Simulations will be conducted on specific known cases of pollution leaks caused by incident fires occurred on industrial or waste treatments facilities.

Passive tracers have no influence on the model itself. Instead, they are strongly influenced by the model output. Tracers are added to the model and WRF blow them around. In other words it is like initiating a puff of smoke at a location at some time and letting the winds blow the smoke around.

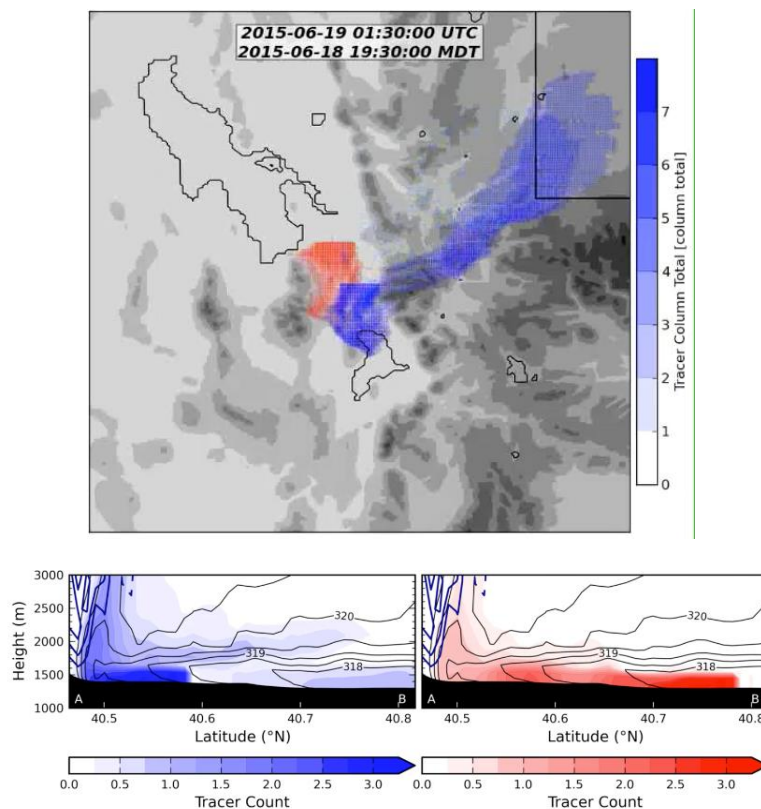


Figure 9 - Example of tracer simulation with the concentration highlighted

Some modification on the core have been applied in order to make the model able to correctly simulate tracers together with the usual output.

As example the event occurred the 11 December 2018 in the northern district of Roma (Salaria) has been simulated using ECMWF ERA re-analysis initialization data and the output of the tracer plume is shown in Figure 10.

Despite no chemical or additional information of the pollutant composition has been inserted, the simulated plume extension and shape is qualitatively in good agreement with the on-ground observations. Further improvements will consist in validating such kind of output with the on-ground measurements performed by the Baquinin network of instruments.

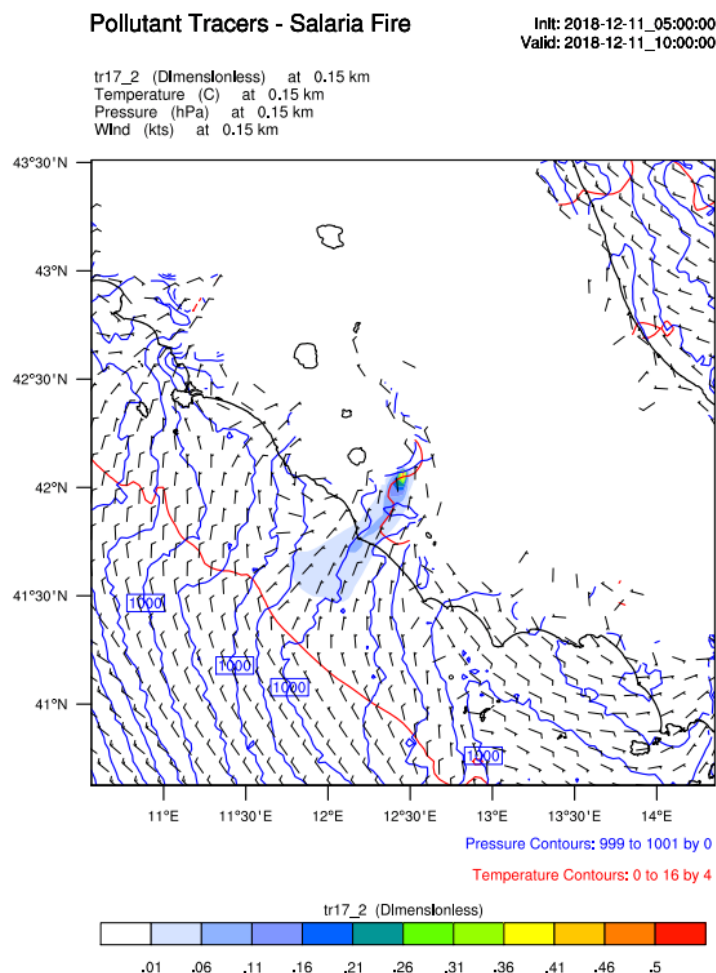


Figure 10 – Plot of the pollutant plume simulated by using WRF output.



Figure 11 - Picture of the event from an on-ground point of view.

This special module can be activated both in real-time mode and in case of re-analysis.