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SEDOO-AERIS

BAMED - BOUNDARY LAYER PRESSURIZED BALLOONS TRAJECTORY SIMULATION

TECHNICAL DOCUMENT
& USER MANUAL

	Name	Organisation	Date	Visa
Written by:	Daria Malik	Magellium	13/10/2023	
Checked by:	Vanessa Pedinotti	Magellium		
Approved by:	Béatrice Berthelot	Magellium		

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Contents

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1. BAMED Overview

BAMED is a Fortran based numeric tool that allows to simulate Boundary Layer Pressurized Balloons (BLPB) trajectories based on the given meteorological conditions. The model allows simulating balloon path from a given launch site (geographical coordinates) on the given date and time of the launch.

All of the BAMED executables and dependencies are wrapped up into a Singularity container.

1.1 BAMED architecture

The BAMED main executable that launches simulations is called traj_blpb and located in the source directory of the tool in the Singularity container : `/usr/local/bamed/src/traj_blpb`

The executable needs as input a configuration file blbp.dat and a file with a list of the ECMWF grib data to use list.dat (Fig. 1). The names of these files are not to change. The traj_blpb can be located anywhere but has to be called from a directory where the two input files are located. The output file blpb_[date]_[hour]_[density]_[number].dat will be written in the directory where the executable is called. One simulation launch can simulate multiple balloons' trajectories with different densities, but same date, time and launch site coordinates (which are defined in the blbp.dat file).

Figure 1 : scheme of the BAMED simulation input/output

1.2 BAMED input files

1.2.1 blbp.dat

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The blbp.dat configuration file contains all of the needed information about the launch and the input meteorological data. The file syntax is as follows :

```
*****************************************
* Input file for the BLBP trajectory model  *
*****************************************

* COMPUTATIONNAL DOMAIN
-10.0                          WEST LONGITUDE (° EAST)
10.0                           EAST LONGITUDE (° EAST)
38.0                           SOUTH LATITUDE (° NORTH)
48.0                           NORTH LATITUDE (° NORTH)
0.1                            GRID SIZE IN DEGREES
48                             NUMBER OF VERTICAL LEVELS
137                            MAX ID NUMBER OF LEVELS
*
* TIME MANAGEMENT
20120911                       START DATE (YYYMMDD)
100000                         START TIME (HHMMSS)
2                              SIMULATION DURATION IN NUMBER OF DAYS
1                              TIMESTEP OF DATA
0.1                            TIMESTEP OF SIMULATION IN HOURS
*
* GRIB DIRECTORY
/home/grib_data                GRIB DIRECTORY
*
* BALOON INFO
1                              NUMBER OF LAUNCH SITES
*
* LAUNCH SITE
4.273968                       SITE LONGITUDE
39.82833                       SITE LATITUDE
1                              NUMBER OF BALOONS
0.95                           FIRST BALOON DENSITY
0.0                            DENSITY RANGE BETWEEN BALOONS
*
```

"Computational domain" block contains the information about the ECMWF grib files that will be used for the simulation : latitude and longitude boundaries of the data, its spatial resolution and information about vertical levels. The last two parameters are the amount of vertical levels contained in files and the maximum ID number of present levels (e.g. if one has data on levels from 10 to 16, the amount of levels is 7 and the maximum ID number is 16).

The "Time management" block contains the information about the simulation start date and time, the simulation duration (in number of days), the timestep of your grib data (in hours), and the timestep of the simulation (in fraction of hour). For example, in the configuration above trajectories will be simulated from 11/09/2012 10:00 until 13/09/2012 10:00 (2 days); the meteorological data provided by the user is an hourly data (one file per

hour); balloons position will be calculated for every 6 minutes (0.1 hour). Logically, the simulation start date and time should be the same as the balloon launch date and time. Here, the balloon is launched at 10:00 on 11/09/2012. N.B: the data timestep is a very important parameter that should be set carefully depending on your available grib data. Based on this value and the duration of simulation the program will search for an exact amount of grib files through the list.dat file. If this operation fails, the simulation is not launched. Furthermore, the timestep between grib data files must be the same.

The "*Grib directory*" must contain the path to the directory with the necessary meteorological data. The path should end with the slash "/".

"*Baloon info*" should always contain "1" for Fortran file reading purposes.

"*Launch site*" block contains information about the launch site (latitude and longitude of the launch position) as well as the balloon configuration (number of balloons, the balloon density and eventual density range). The parameter "number of balloons" has priority over the "density range"; it means that even if the density range is different from zero but the number of balloons is equal to 1, then only one balloon with the "first balloon density" will be simulated. In case of more than one balloon, their respective densities will decrease from the initial density by the density range step (examples in the Table 1 below). Regardless of the number of balloons, the launch coordinates will be the same for all of them for a one given blbp.dat configuration.

Table 1 : Examples of different density configurations

Number of balloons	Initial density	Density range	Densities of simulated balloons
1	0.95	0.0	0.95
1	0.95	0.1	0.95
2	1.00	0.05	1.00, 0.95
4	1.10	0.1	1.10, 1.00, 0.90, 0.80

1.2.2 list.dat

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The list.dat file should contain the list of the meteorological grib files needed for the simulation. The user has to make sure that the data listed in this file is consistent with the simulation configuration (temporal and spatial cover).

The format of the list.dat is as follows (example below) :
- date of the data in YYYYMMDD format
- two spaces
- time of the data in HHMMSS format
- two spaces
- name of the corresponding file in YYMMDDHH.grib format

```
   20230206   000000   23020600.grib
   20230206   030000   23020603.grib
   20230206   060000   23020606.grib
   20230206   090000   23020609.grib
   20230206   120000   23020612.grib
   20230206   150000   23020615.grib
   20230206   180000   23020618.grib
   20230206   210000   23020621.grib
   20230207   000000   23020700.grib
   20230207   030000   23020703.grib
   20230207   060000   23020706.grib
   20230207   090000   23020709.grib
   20230207   120000   23020712.grib
   20230207   150000   23020715.grib
   20230207   180000   23020718.grib
   20230207   210000   23020721.grib
   20230208   000000   23020800.grib
```

1.3 BAMED Output Files

BAMED outputs balloons' trajectories in the ASCII format with semicolon separator. There is one .dat file per balloon. The output name is always in the blpb_[date]_[hour]_[density]_[number].dat format. The file itself contains following information :

```
launch_lat;44.4680000000
launch_lon;11.3240000000
launch_date;20230701
launch_time;030000
density;0.900
Variables:;time;longitude;latitude;altitude;vertical_velocity;total_precipitation
Units:;seconds;degrees_east;degrees_north;meters;Pa/s;meters
;360.00;11.30015857;44.46197394;2751.19;-.48956685;.00065226
;720.00;11.27665363;44.45572407;2746.49;-.46246899;.00068714
```

```
;1080.00;11.25351685;44.44912894;2736.90;-.42619016;.00074184
;1440.00;11.23072450;44.44204434;2721.75;-.38302931;.00078967
;1800.00;11.20819935;44.43430726;2700.33;-.33591633;.00081080
;2160.00;11.18580403;44.42573992;2671.75;-.28843430;.00079018
;2520.00;11.16333724;44.41616158;2634.78;-.24597784;.00072275
;2880.00;11.14052695;44.40542292;2588.68;-.21542174;.00064191
;3240.00;11.11702922;44.39343465;2532.60;-.20389508;.00059015
;3600.00;11.09245787;44.38019171;2465.33;-.21609697;.00061181
end_status;0
```

The header of the file allows to keep track of the launch information : launch position (latitude, longitude), launch date and time as well as the balloon density. Some of this information is also present in the name of the output file.

The time, latitude, longitude and altitude column contain the balloon estimated position information. The columns vertical velocity and the total precipitation are estimated only if these variables are also present in the ECMWF input meteorological files. These variables are not mandatory at input, and it does not impact the results of the simulation. If they are not present, the values in the output file will simply be written "0.00".

The last line of the file contains the exit status of the simulation :
- 0 = launch site (before the simulation) is outside of the geographical domain or balloon position (during simulation) exits the geographical domain before the requested duration of simulation were reached
- 1 = simulation successful
- 4 = balloon exits through domain bottom-level
- 5 = balloon exits through domain top-level
- -9= density warning, two last estimated balloon positions are identical

In all of the above cases an output file is created even if no balloon position were estimated.

2. BAMED simulation for User
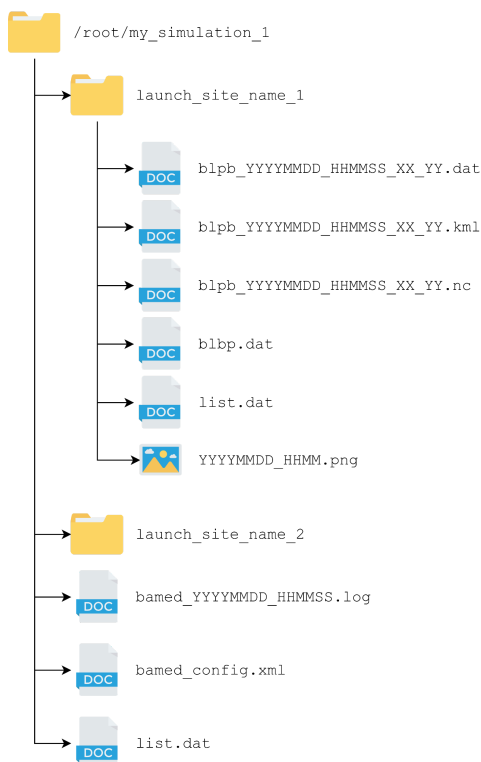
2.1 BAMED Singularity container

Figure 2 : Folder structure for one simulation

BAMED code is containerized into a Singularity container, which allows any user to run it without previous libraries installation and Fortran configurations (except the installation of the Singularity application itself).

2.2 BAMED User interface

The user interface for the easier simulation launches is a Python script which requires a special XML configuration file from the user, but then the script takes care of writing BAMED input .dat files, looping through multiple simulations if needed, launching the simulation itself and creating additional output files for users. This Python code must be executed inside of the BAMED Singularity container.

Python script requires an XML configuration file where principal simulation parameters are defined by the user. After the simulation is done, the code takes the ASCII output from Fortran and recreates it in different additional formats for future user's analysis. For each launch site and launch datetime, additional outputs from Python script are :

- PNG plot of the estimated balloon trajectories overlaid on a map
- KML file with balloon positions for a quicker visualization in GIS applications
- netCDF file with ballon positions and launch information

An example of the directory structure with input and output files for a simulation is presented on Fig. 2. Directories `launch_site_name_1` and `launch_site_name_2`

were created by the Python script based on the user configuration where two launch sites were requested, respectively with names "*launch_site_name_1*" and "*launch_site_name_2*". For each launch site, there will be output .dat, .kml and .nc files, as well as png plots for each launch dat/time requested in the configuration file (example of a plot on Fig .3).
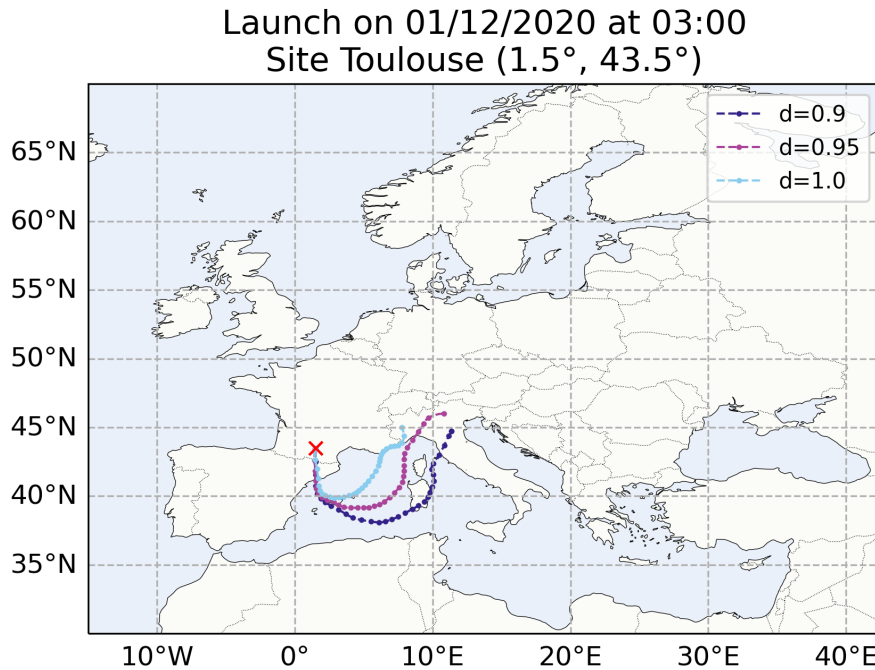

Figure 3 : plot of estimated balloon positions for a launch at (1.5°E, 43.5°N) coordinates, on 1st of December 2020 at 03:00 UTC; balloons have density of 0.9, 0.95 and 1.0 respectively

2.2.1 User configuration file

User configuration file is an XML file where it is possible to set up multiple different variables and parameters of the simulation.

The node `<launch>` allows configuring multiple date and times of launch as well as multiple launch sites. The node `<date>` allows to indicate one or multiple dates (separated by a slash) where the simulations must be performed, and the node `<time>` allows to configure one or multiple times (separated by a slash) for previously requested dates. The simulation will be performed for each possible date/time combination. *The datetimes of launches have to match the datetimes of available meteorological data.*

The `<launch_site>` node allows you to configure one or multiple launch sites. There has to be only one `<launch_site>` node, but inside this node each child

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<site> node will correspond to one distinct launch place. The syntaxe is <site name="my_site"> latitude_value / longitude_value </site>. The attribute name in the node must be different for each site because these names will be also used to create output directories for each launch site. Simulations of each of the sites will run for every launch datetime configured earlier in the file. The longitude values can be either in the [-180°;+180°] or [0°;+360°] convention, but this convention must be the same as the one used for the simulation geographical extent.

The node <balloons> allows to set up the values of the balloons densities. The syntaxe is <density> density_value_1 / density_value_2 / density_value_3 / etc </density>.

```xml
<launch name="launch-1">
    <launch_datetime>
        <!-- launch date (YYYYMMDD) -->
        <date>20230701/20230702</date>
        <!-- launch time(s) HHMM, separated by a slash in case of multiple times -->
        <time>0900/1200</time>
    </launch_datetime>
    <launch_site>
        <!-- launch site latitude, longitude in "lat/lon" format for each desired site -->
        <!-- names matter only for the output/input folders distinction, they should be different -->
        <site name='site-1'> 44.468 / 11.324 </site>
    </launch_site>
    <baloons>
        <!-- baloon densities -->
        <density>0.90/0.95/1.00</density>
    </baloons>
</launch>
```

Figure 4 : bamed-config.xml file example, <launch> node

The <simulation> node allows configuring simulation geographical and temporal extent. The <grib_time_step> node indicates the timestep between your input ECMWF data files. The longitude values can be either in the [-180°;+180°] or [0°;+360°] convention, but this convention must be the same as the one used for the launch sites coordinates.

```xml
<simulation>
    <!-- Latitude/longitude simulation extent -->
    <lat_min>30</lat_min>
    <lat_max>60</lat_max>
    <lon_min>0</lon_min>
    <lon_max>30</lon_max>
    <!-- Simulation duration (in days) -->
    <duration>3</duration>
    <!-- simulation timestep in seconds (maximum 360 secs) -->
    <time_step>360</time_step>
    <!-- timestep of the grib data in hours -->
    <grib_time_step>3</grib_time_step>
</simulation>
```

Figure 5 : bamed-config.xml file example, <simulation> node

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The `<paths>` node indicates the script where to search for the input data, and where to store working and output files.

```xml
<paths>
    <!-- path to the directory where grib files are stored -->
    <grib_path>/my_data_ecmwf/bamed/2020</grib_path>
    <!-- path to the directory where working files for the simulation will be stored -->
    <working_path>/home/work/bamed/simu_1</working_path>
</paths>
```

Figure 6 : bamed-config.xml file example, <paths> node

Two different simulation scenarios (meaning simulations with two different XML configuration files) can be performed simultaneously but in different working directories. Otherwise, the first simulation must be finished before launching the next one.

2.2.2 Python simulation launch script

Python script constitutes a link between user configuration file and the BAMED executable in the Singularity container. The script reads the XML configuration file, and manages all of the simulation combinations : writing input .dat files for BAMED, launching simulation, output log messages in a log file, creating figures for a quick and easy visualization of results, and transforming output results into the KML and netCDF formats in addition to a default ASCII output of the executable.

The Python interface takes as input two arguments : file path to the configuration file (mandatory) and the shell log output argument (optional). If the shell log argument is not provided, then the output log is only written into the log file. If the option is provided, the output log is also displayed simultaneously on the screen.

```
usage: bamed.py [-h] [-bc CONFIG] [--shell-log]

This Python script allows to manage multiple BAMED simulations based on the
user configuration XML file

optional arguments:
  -h, --help              show this help message and exit
  -bc CONFIG, --config CONFIG
                          Filepath to the xml configuration file (mandatory)
  --shell-log             Provide this argument if you want to display log
                          messages on the screen in addition to the log file
```

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2.3 BAMED simulation launch

The python script has to be executed *inside the Singularity container* with the BAMED code. There are multiple methods to do so.

2.3.1 Interactive launch

If you want to launch the simulation in the interactive mode and be able to continue to work in the Singularity container, you can follow these steps:

1. launch Singularity container in the shell mode

```
singularity shell path/to/the/container.sif
```

2. launch Python script with log messages display

```
python3 /my/path/bamed.py \
-bc /path/to/the/bamed-config.xml \
--shell-log
```

or without messages display (only log text file)

```
python3 /my/path/bamed.py \
-bc /path/to/the/bamed-config.xml
```

If the input data or your working directory are not exactly directories owned by your user, or can't be seen by the container (for example, if you are performing simulations on a server with multiple users and shared folders and volumes), you might need to bind these directories to the container with the `--bind` option. After the `--bind` keyword you can list separated by commas *absolute paths* to the folders that you would like to be seen by the Singularity container :

```
singularity shell --bind /root/input_data/,
/home/working_folder/simu_xx path/to/the/container.sif
```

Based on your host system, most of the field and folders owned by your user will be seen, but sometimes special access may be required, and the `--bind` option can help you to link these folders to your container.

2.3.2 Non-interactive launch

It is also possible to launch the script in one go with the singularity exec command :

```
singularity exec path/to/the/container.sif python3 \
/my/path/bamed.py -bc /path/to/the/bamed-config.xml [--shell-log]
```

The --bind option can be used here in the same manner as in the example above with `singularity shell`.

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All of the methods described above can be wrapped into cron, bash scripts or slurm jobs depending on one's needs and number of simulations.

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3. ECMWF data extraction for BAMED with automatic simulation

It is possible to extract the ECMWF data for the BAMED simulation and to launch the simulation right afterwards on a distant server via a bash script bamed_extract_ecmwf.sh which prepares the data extraction and then launches the simulation remotely on a user's requested server. This script has to be launched on one of the ECMWF MARS servers, as it uses the MARS API for meteorological data extraction.

The script contains three main parts :

1. prepare MARS requests for the data extraction
2. send the data to the distant server indicated by user
3. launch simulation remotely on this distant server

Some simulation parameters must be provided by the user in order to configure the data extraction and the simulation. With a certain configuration it is also possible to perform only the data extraction, without data transferring nor simulation. These possibilities will be detailed below in the rest of the chapter.

Following parts of this chapter describes in detail what data is needed by the simulation, how to extract the data with the given script, and how to make it launch simulations automatically as soon as the data extraction is finished.

3.1 Data fields and format

The ECMWF data for the BAMED simulation has to be organized in a certain manner: all variables for the same date and time should be packed together in one file. The mandatory meteorological fields are:

- U component of wind (U)[1]
- V component of wind (V)
- specific humidity (q)
- temperature (t)
- logarithm of surface pressure (lnsp)
- vertical velocity (w)
- total precipitation (tp)

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[1] the short name of the field in the parentheses corresponds to the short name of this field in the ECMWF MARS database

All of the variables, except the logarithm of surface pressure, are level variables. An example of the grib_ls command on one of the files is presented on Fig. 7 below.

edition	centre	date	dataType	gridType	stepRange	typeOfLevel	level	shortName	packingType
2	ecmf	20140606	an	regular_ll	0	hybrid	98	u	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	99	u	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	98	v	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	99	v	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	98	t	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	99	t	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	98	q	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	99	q	grid_simple
2	ecmf	20140606	an	regular_ll	0	hybrid	1	lnsp	grid_simple

Figure 7 : example of grib_ls command output for the BAMED ready meteorological grib file

The data should cover the desired time of your simulation, *and* be extended 1 day before and after the simulation. For example, if your simulation period is from 5th to 7th of March 2021, the data should cover the time period from 4th to 8th of March 2021. The script will take care of these extensions, so in the input configuration you should define your true simulation time period, without taking into account this +- 1 day surplus.

3.2 Input parameters configuration

The script takes as input a configuration txt file. This configuration file contains all the parameters that the user can change and configure:

```
# Data configuration
ID_NAME="palavas_campaign"
START_DATE=""
N_DAYS=2
GRID_RESOLUTION="0.1"
LAT_MIN="26.56"
LAT_MAX="28.92"
LON_MIN="6.02"
LON_MAX="10.00"
WORKING_DIR="/home/user/bamed"
DATA_DIR="/root/data/bamed_data"
USER_EMAIL="user@mail.com"
SERVER_USER="remote_user"
SERVER_ADDRESS="remote.server.com"
SERVER_DATA_DIR="/remote_root/remote_bamed_data"
# Simulation configuration
LAUNCH_DATE="20230701"
LAUNCH_TIME="0300/0900/1500"
LAUNCH_SITE_NAME="Italy/Germany"
LAUNCH_LAT="44.468/48.503"
LAUNCH_LON="11.324/9.246"
BALOONS_DENSITY="0.90/0.95/1.00"
SIMULATION_DURATION="3"
```

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```
SIMULATION_TIMESTEP="360"
SERVER_WORKING_DIR="/remote_root/remote_bamed_working_dir"
```

The *ID_NAME* parameter can be a name or an ID character sequence that will allow you to distinguish between your different data requests. Along with the log file of your request that will contain this ID name in the filename, the directory with your corresponding data will also be entitled with this ID.

The *START_DATE* corresponds to the start date of the time period for which you would like to extract the data. This date can be anything up until the current day's date and you can also leave it empty. Leaving it empty is equivalent to putting a "today" date.

The *N_DAYS* value is a number of days in your time period or which you would like to extract the data. Note, that the maximum forecast period is 10 days (D+240h). Based on the starting date and the duration of the extraction, if the requested dates are in the past or past+future, the data timestep will be of 3h. The "past" part will have the analysis fields every 6h and the filling of 3h is done with the forecast fields of the corresponding date. The "future" part will be the forecast fields of every 3h. However, if the requested data is only in the future (forecast only), the step is adapted based on the ending date of the request: 1h step if up to +90h, 3h step up to +144h and 6h step for up to +240h. This variable timestep in the forecast data is governed by the ECMWF.

The parameters *GRID_RESOLUTION* and *LAT[LON]_MIN[MAX]* allow the user to configure the geographical extent and spatial resolution of the data. It is important to note that the values of the lat/lon are the boundaries of your ROI and not the coordinates of boundary pixels' centers.

The *WORKING_DIR* parameter corresponds to the directory on the MARS server where the ID directory for the extraction will be created in order to store the working files.

DATA_DIR is the directory on the MARS server where the final data will be stored. Depending on the volume of data, you should consult the documentation [1] to find a suitable directory based on its available free disk space.

SERVER_USER[ADDRESS][DATA_DIR] allows you to send the data onto your local server where you would like to store the data and run simulations. The script anticipates the ssh-copy-id command to establish the password-free connection between the MARS and your final server for the data transfer. If this command has never been executed before, first launch could ask you for your password in order to initiate the automatic authentication. These parameters can also be left empty. In this case, no files will be transferred, you can find the data in your data directory of the MARS server.

LAUNCH_DATE[TIME][SITE_NAME][LAT][LON], *BALOONS_DENSITY*, *SIMULATION_DURATION[TIMESTEP]* and *SERVER_WORKING_DIR* are parameters that will be

.

used in the XML configuration file for the BAMED Python script described in the previous chapter. Multiple launch dates (and times) can be configured via writing required dates (or times) separated by the slash. The code will then run simulations for every combination of launch date/time. Same method can be applied to multiple density values configuration and the launch sites. For the launch sites, names, latitudes and longitudes are each separated by the slash in the respective variable setting in the parameter file. *SERVER_WORKING_DIR* is a remote directory where the simulation will be run.

If all the parameters are set properly, then the script will perform all of the steps as indicated in the introduction of this chapter: extract the ECMWF data, send it to your "working" server, prepare the Python configuration file and launch Python inside the singularity container. The log messages of an eventual error or warnings will be logged in log files or displayed on the screen. Two cases are offered to the user :

- set all the parameters correctly and get the extracted data and performed simulation

or

- do not set parameters *SERVER_USER[ADDRESS][DATA_DIR]* in order to only extract the meteorological data from the server, and not perform simulation nor data transferring to the distant server. The extracted data is perfectly suitable for subsequent simulations.

The only parameter that you must change in the script itself if you want it to launch simulations automatically, is the path to the Singularity container and the bamed.py user script on your distant server. The Python script and the Singularity container can be located anywhere independently of your working or data directories.

```
72   SING_CONTAINER_PATH="/home/user/BAMED/src/bamed.sif"
73   PYTHON_PATH="/home/user/BAMED/src/bamed.py"
```

Figure 8 : lines to be changed in the data extraction script

2.3 Data and folder organization

The structure of your working and data folders is summarized on Fig. 8. For a given campaign and a start date with N days duration, the folder "`campaign_name`" with a folder "`<start_date>_<end_date>`" inside it will be created in your working directory, and the same thing will be created in the data directory as well.
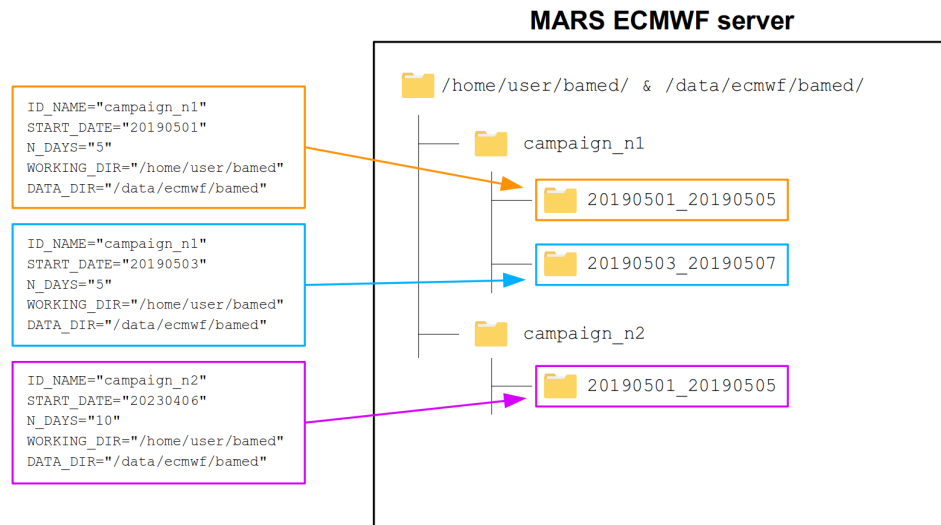
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MARS ECMWF server

Figure 9 : user's folder organization of different simulations on the MARS server

2.4 Data extraction launch

To extract the data, you should follow next steps:

1. log in to the ECMWF MARS server
2. set up parameters in your configuration file [.conf]
3. do : `path/to/the/bamed_extraction.sh --config \`
   `path/to/the/conf_file.conf`

The script will launch the extraction based on your set up parameters, and then continue with the data copy and simulation launch. It is advised to launch this script as a SLURM job on the MARS server, otherwise the shell will be inaccessible and the script might take longer to perform. To launch this script as a job, you can use the following syntax :

```
sbatch --wrap="path/to/the/bamed_extraction.sh --config \
path/to/the/conf_file.conf"
```

This command will launch a SLURM job with your configuration file and create a .out log file in the directory from where the command was called. You can consult the SLURM documentation [2] to see how you can customize this call and add features like job name or mail user for notifications.

In the end of the extraction and file formatting the data will be transferred to your server (if indicated), and you will receive an email notification that the job has been

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completed, if you enabled the mail notifications of the job [2]. The job can exit if an error occurs during the data extraction, data transfer or simulation job submission. If the simulation itself has not succeeded, you should check the simulation log output on your distant server to investigate the error.

References

[1] ECMWF MARS server filesystems

https://confluence.ecmwf.int/display/UDOC/HPC2020%3A+Filesystems

[2] SLURM sbatch command input options

https://slurm.schedmd.com/sbatch.html

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