MODEL CHAIN FOR BUOYANT PLUME DISPERSION.

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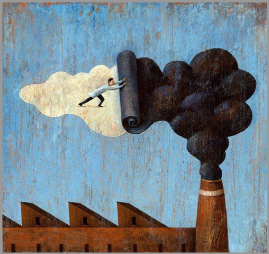
Talk outline

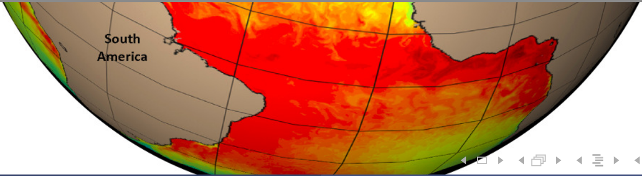
- Overview of the Model Chain:
  - WRF, the Weather Research and Forecasting Model;
  - SPRAYWEB the Dispersion Model.
- WRF-SPRAYWEB Interfacing.
- Comparing simulation for EPRI BULL RUN Data Set including:
  - Meteorological Data;
  - Statistical Indexes for Concentration Field.



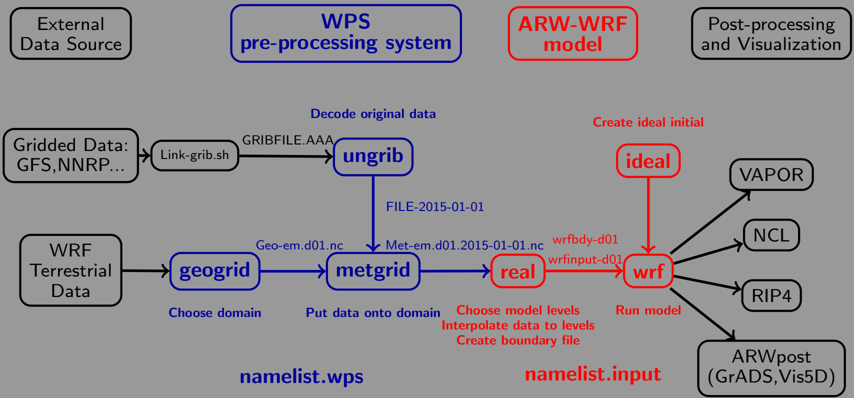
Weather Research and Forecasting (WRF) Model

The WRF-ARW model is a fully compressible, nonhydrostatic model with terrain-following hydrostatic pressure vertical coordinate. It contains initialization programs, a numerical integration program and a program to do one-way nesting, and it supports a variety of capabilities including:

- The grid staggering is an Arakawa C-grid.
- Runge-Kutta 2nd and 3rd-order time integration schemes.
- 2nd to 6th-order advection schemes.
- Time-split small step for acoustic and gravity-wave modes.
- The dynamics conserves scalar variables.
- Real-data and idealized simulations.
- Various lateral boundary condition options.
- Full physics options.
- One-way, two-way nesting and a moving nest.
- Applications ranging from meters to thousands of kilometers.



WRF Work Flow



Particles Lagrangian Stochastic Models LSMs

Basic assumptions

- Emissions in the atmosphere are simulated using a certain number of **fictitious particles**.
- Each particle represents a specified pollutant mass.
- The time evolution of a fluid particle velocity in a turbulent flow can be considered as a **Markov process**.

Langevin equation (Stochastic Differential equations SDE)

$$du_i = a_i(\vec{u}, \vec{x}, t)dt + b_{ij}(\vec{u}, \vec{x}, t)dW_j$$
$$dx_i = (u_i' + U_i)\,dt$$

where

- $a_i(\vec{u}, \vec{x}, t)$ is the drift coefficient, a deterministic term.
- $b_{ij}(\vec{u}, \vec{x}, t)$ is the diffusion coefficient.
- dW_j is the increment of a Wiener process whose distribution is $G(0, dt)$.
- $b_{ij}(\vec{u}, \vec{x}, t)dW_j$ represents the random stochastic term.

SPRAYWEB

SPRAYWEB (Tinarelli et al, 1994; Alessandrini and Ferrero, 2009; Alessandrini et al. 2013) is a LSM designed to study the pollutants dispersion in complex terrain.

- In the two horizontal directions the PDF is assumed to be Gaussian.
- In the vertical direction the PDF is assumed to be non-Gaussian, so to deal with convective conditions.
- The equations prescribing the evolution of the vertical velocity fluctuation w and the displacement z are the following:
  - $dw = a(z, w)dt + \sqrt{C_0 \epsilon} dW$
  - $dz = wdt$
- $a(z, w) = \frac{1}{P}\left(B_0 \frac{\partial P}{\partial w} + \Phi\right)$ is determined by solving the Fokker-Planck equation,obtaining: where P(z ,w) is the PDF.
- In the present work we used the Gram-Charlier PDF (Ferrero and Anfossi, 1998).
- SPRAYWEB includes the method for the buoyant plume rise simulation proposed by Anfossi et al. (1993).

WRF-SPRAYWEB Interface: Vertical coordinate

SPRAYWEB

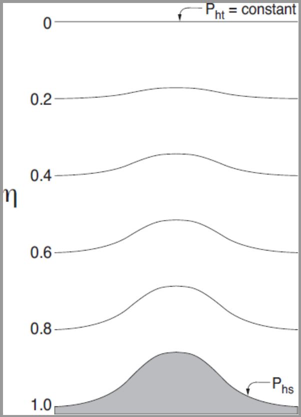
- **Terrain-following coordinates** (x, y, s) to express the orography.
- They are related to the cartesian coordinates (x, y, z) as:
  $x = x$
  $y = y$
  $$s = \frac{z - z_g(x, y)}{z_t - z_g(x, y)}$$
  z_t is the top of the domain and $z_g(x, y, z)$ is the orography
- e.g. $s = 1$ for $z = z_t$ and $s = 0$ for $z = z_g(x, y)$ so that $s = 0$ is not a horizontal plane but the orographic surface.

→ Time independent mapping from η to s

WRF

- **Terrain-following hydrostatic-pressure coordinates** (Laprise 1992) defined as:
  $$\eta = \frac{p_h - p_{ht}}{p_{hs} - p_{ht}}$$
- p_h is the hydrostatic component of the pressure, p_{hs} and p_{ht} refer to the values along the surface and top boundaries respectively.
- η definition is analogous to σ coordinate but η varies from a value of 1 at the surface to a value of 0 at the upper boundary.
- η are also called **vertical mass coordinate** and they are **time-dependent**.

WRF-SPRAYWEB Interface: interpolation procedure



- We choose a certain η at fixed time,
- We choose the time step in which the η **coordinate reaches the maximum height**, so that all the other $\eta(t)$ can be interpolated on this one without exceed the domain.
- We **interpolate all the time-dependent WRF output variables on this given** η
- η decreases with the height while *s* increases, hence we need to **invert the interpolation** by considering $1 - \eta$ instead of η
- We perform the **cubic spline interpolation** of Forsythe, Malcolm and Moler (1977) in which an exact cubic is fitted through the four points at each end of the data, and this is used to determine the end conditions.

WRF-SPRAYWEB Interface: Turbulence parameters

Estimate the Obukhov length from the three WRF output variables:

- HFX, the heat flux at surface.
- T2, 2-meters temperature.
- UST, the frictional velocity computed using similarity theory.

Evaluate the turbulence parameters through **Hanna (1982) parameterisation** by using:

- the Obukhov length
- the WRF output variables PBLH, i.e. the Atmospheric Boundary layer thickness
- the convective vertical velocity parameterised ad function of PBLH, T2, HFX

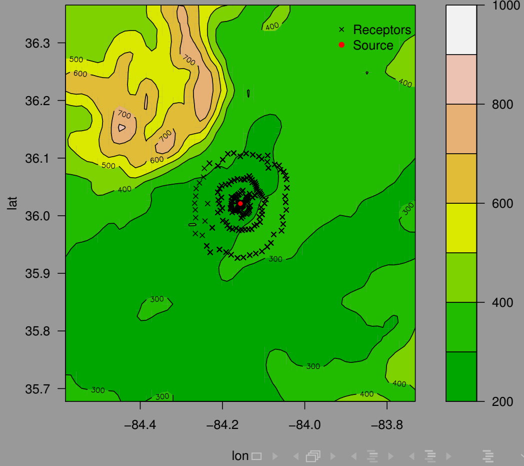
Interpolate the turbulent parameters:

- the velocity standard deviations $\sigma_x, \sigma_y, \sigma_z$
- the Lagrangian scale times T_u, T_v, T_w

EPRI Bull Run Experiment

Bull Run Dataset (Hanna and Paine 1989)

- Study period August-October 1982
- Moderately hilly site near Oak Ridge, Tennessee
- SF6 emissions from a 244 m stack
- Hourly measures of ground level concentrations
- Network of about 200 monitors
- Monitors spaced on arcs at downwind distances ranging from 0.5 to 50 km
- The arcs extended completely around the stack



Simulation settings

WRF

- Simulation time period: from 00:00:00 15/10/82 to 00:00:00 16/10/82
- Interval 21600 second
- 4 horizontal nested grids with parent ratio 3
- Number of grid points 33, 133, 133, 67
- Extension of grids 3960 km, 1320 km, 440 km and 73
- Horizontal resolution 30000 m, 10000 m, 3333 m and 1111 m
- Integration time steps for the 4 grids: 90 s, 30 s, 10 s, 3 s
- Stretched grid in vertical direction of 38 levels from $\eta = 1$ to $\eta = 0$
- Meteorological input NNRP data, the NCEP/NCAR reanalysis with a resolution of 2.5 deg, a six hours output frequency , 17 pressure levels
- 27 incoming vertical levels (it is determined by the NNRP data)

Simulation settings

SPRAYWEB

- Simulation time period 14-23 (LST), 15th October 1982
- Ground level concentrations measured:
  - at the three arcs with radius 2, 5, 10 km as in Hanna and Paine (1987)
  - for time period 15-18 as in Hanna and Paine (1987)
- Simulation time step 30 s
- Starting step and frequency 1800 s
- Minumum emission spacing 5 s
- Grid step on x and y direction 720 m
- Number of grid points in x,y,z direction: 100,100,20
- Top of concentration domain 5000 m
- PBL height 1000 m
- Height of first layer 40 m

Some WRF physics and dynamics options

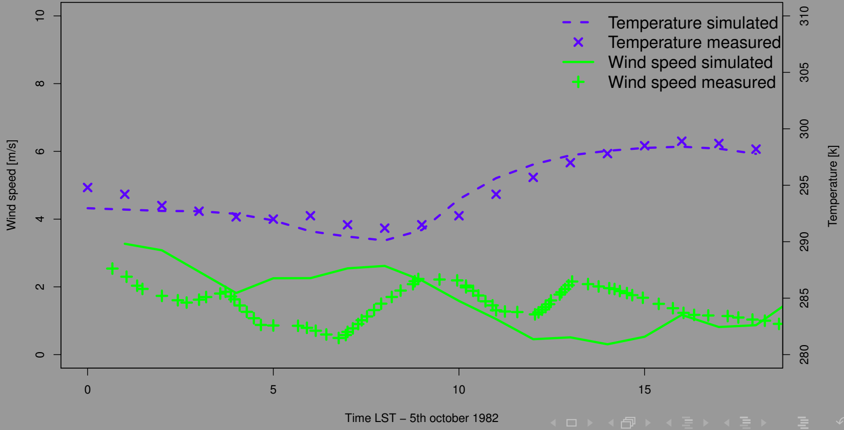
Physics options in namelist.input

- mp-physics=4
  use of WSM 5-class scheme as microphysics option
- sf-sfclay-physics=1
  Monin- Obukhov similarity theory as surface scheme
- sf-surface-physics=2
  Noah Land Surface Model for the surface physics
- bl-pbl-physics=1
  YSU PBL scheme for the PBL parameterization

Dynamics options in namelist.input

- diff-opt=1
  simple diffusion: gradients are simply taken along coordinate surfaces
- km-opt=4
  2d Deformation: K for horizontal diffusion is diagnosed from just horizontal deformation and the vertical diffusion is assumed to be done by the PBL scheme
- non-hydrostatic=true
  Run the model in non-hydrostatic mode

Meteorological Data: comparison beetwen wind speed and temperature simulated with WRF and measured at 100 m height by the meteorological tower during the simulation.



Statistical Indexes for Concentration Field

We compare the maximum and the crosswind integrated concentrations at ground, on the three arcs with radius 2, 5, 10 km in term of the following statistical indexes: mean, correlation coefficient (COR), normalised mean square error (NMSE) and fractional bias (FB).

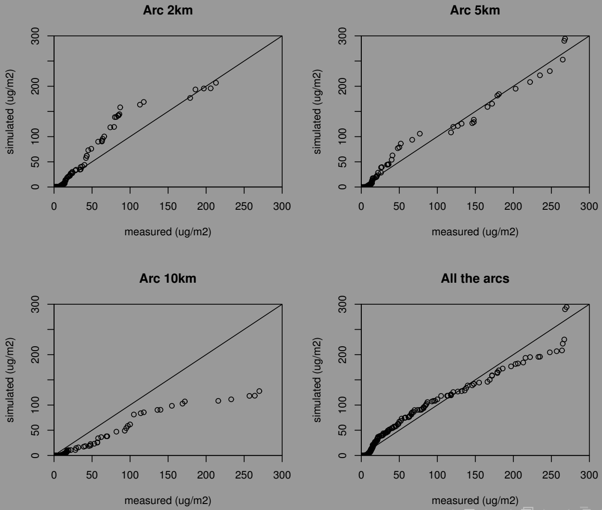
Maximum of ground level concentration

	Mean(μ/m^2)	CORR	NMSE	FB
Measured	256.333	1.000	0.000	0.000
Simulated	288.714	0.928	0.017	0.119

Crosswind integrated concentration

	Mean(μ/m^2)	CORR	NMSE	FB
Measured	6625.421	1.000	0.000	0.000
Simulated	5149.403	0.903	0.219	-0.250

qqplot for crosswind-integrated concentrations



Conclusion I

- The use of WRF as input for SPRAYWEB lead to a series of advantages:
  - WRF model is designed to be a flexible, state-of-the-art, portable code that is efficient in a massively parallel computing environment
  - It offers numerous physics options, thus tapping into the experience of the broad modeling community
  - It is suitable for use in a broad spectrum of applications across scales ranging from meters to thousands of kilometers.
- The meteorological data from WRF are in agreement with the measurements of Bull Run experiment.

Conclusion II

- The statistical indexes from SPRAYWEB for concentration field exhibit a good agreement between the measures and the simulation results:
  - The correlation is very high both for the maximum of concentration at ground and the crosswind integrated concentration.
  - The normalised mean square error is smaller for the maximum of ground level concentration but the value for the crosswind integrated concentration is acceptable as well.
  - The fractional bias shows a slight overestimation for the maximum and an underestimation for the crosswind integrated concentration.
- We show that the two distributions of measured and simulated crosswind integrated concentration can be compared by plotting their quantiles against each other. In particular:
  - For arc with radius 2 km the simulation overestimates the crosswind integrated concentration in range $50\mu g/m^2 - 150\mu g/m^2$, while the two distributions are ver similar for the other values.
  - For arc with radius 5 km the simulation overestimates the crosswind integrated concentration in range $50\mu g/m^2 - 100\mu g/m^2$ and slightly undestimates in the remainder of the range.
  - For arc with radius 10 km the simulation underestimates the crosswind integrated concentration for all the quantiles, expecially for values greater than $100\mu g/m^2$.
  - Overall, the two distributions compare well with a little underestimation for the values up to $120\mu g/m^2$ and an overestimation for larger values.

Work in progress

Further developments would include the following features:

- several PBL schemes available in WRF will be tested in order to understand which one is the most appropriated to build the model chain with SPRAYWEB
- different turbulence parameterisation will be implemented in the interface code.
- new plume rise schemes (Alessandrini et al., 2013; Bisignano and Devenish, 2015) will be developed in SPRAYWEB.

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