FLEXPART training course 2013: Versions

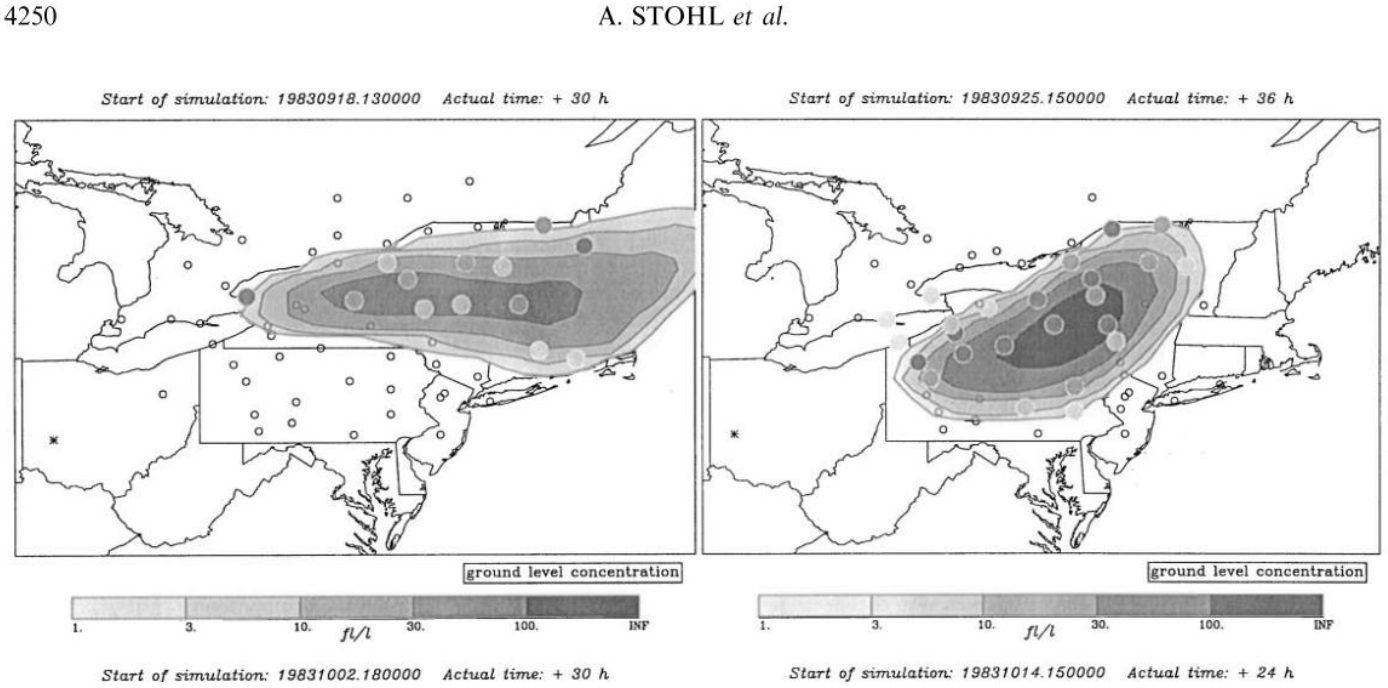
D. Arnold[a] with input from many others

[a] Zentralanstalt für Meteorologie und Geodynamik (ZAMG), Vienna, Austria

Versions and FLEXPART evolution

é starts

Stohl, A., M. Hittenberger, and G. Wotawa (1998): Validation of the Lagrangian particle dispersion model FLEXPART against large scale tracer experiments. Atmos. Environ. 32, 4245-4264.

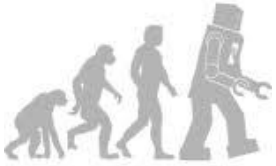


FLEXPART against CAPTEX

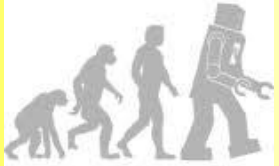
Versions and FLEXPART evolution

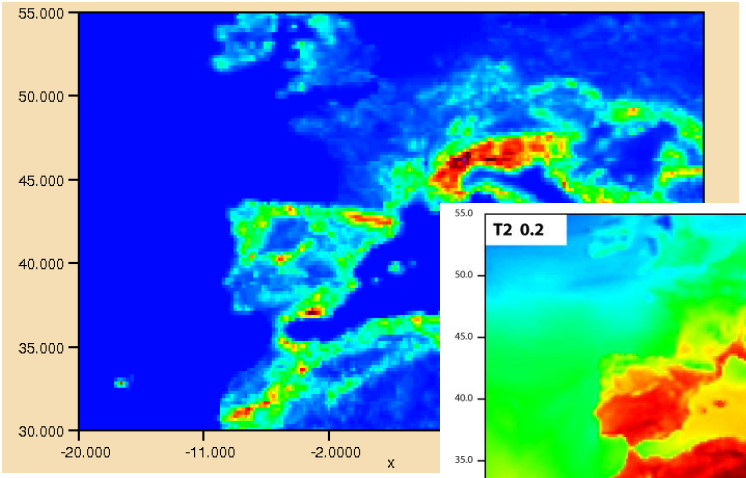
é 5.X → 6.2 → 8.23 → 9.X →

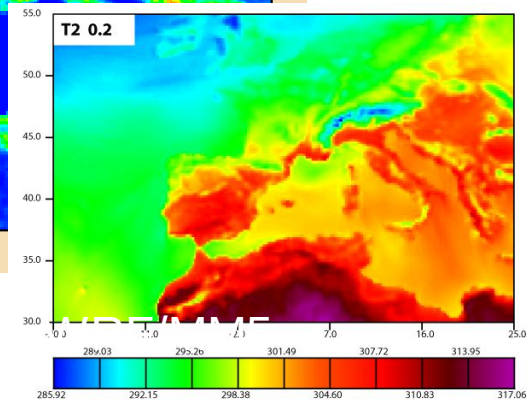
Plus a gfs version

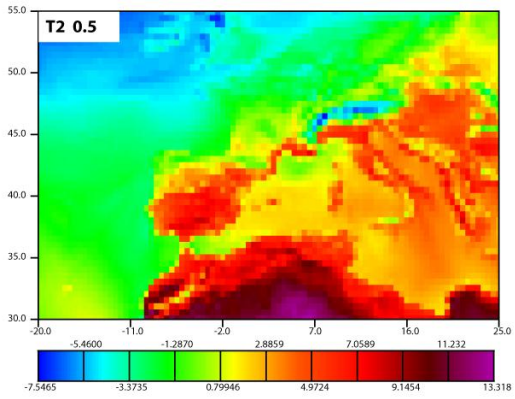


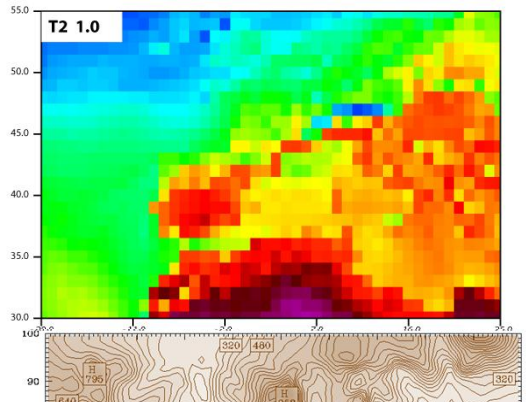
flexpart.eu

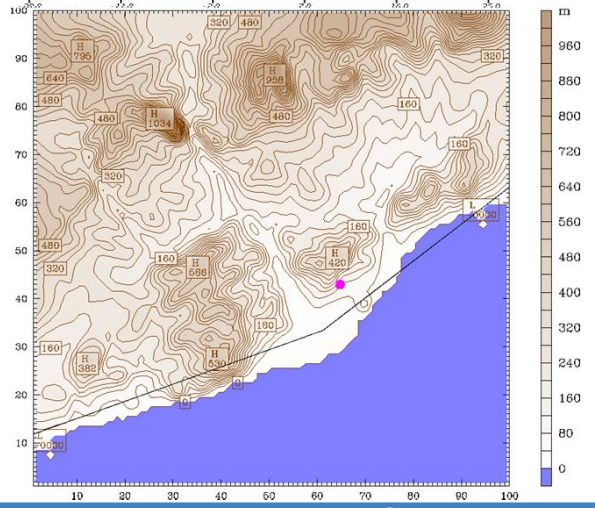












The resolution issueé

Versions and FLEXPART evolution

é 5.X → 6.2 → 8.23 → **flexpart.eu** → 9.X →

Plus a gfs version

6.2 ï MM5 *Seibert and Skomoroski 2004*

6.2 ï WRF (PILT) ***ï*** *Fast and Easter 2006*

6.2 FLEXPART-ALADIN (ZAMG) → conversion of ALADIN output to netCDF needed

9.02 ï WRF, parallel *(Brioude et al. 2013* ***ï*** *soon released)*

9.0x FLEXPART-COSMO (Brunner, Henne, Kaufmann 2013)

Versions and FLEXPART evolution

Version 8.x ï Version 6.2

http://transport.nilu.no/flexpart/flexpart-changes-log-from-version-8-0-to-8.2/view

- Compacted binary output format
- Options/SPECIES/SPECIES_XXX
- Fortran 77 + some introduced Fortran 90 features
- New wet deposition scheme ï in cloud and below cloud scavenging separately
- Added routines and makefiles in the Src for GFS input data
- Input may be in GRIB1 or 2
- Able to use grib_api
- Change in the dynamic viscosity for large Reynolds numbers
- Added switch off kernel near the source

- Sparse/no-sparse matrix binary format
- Options/SPECIES (one single file)
- Fortran 77
- Wet deposition scheme ï in cloud and below cloud scavenging treated in a bulk parameterized form
- No GFS data (Special 6.4 version for this)
- Input in GRIB1
- Using libgribex/libemos
- Documentation included with source code with a very useful flux diagram of the routines

Versions and FLEXPART evolution

Version 9.02 ï Version 8.23

- Fortran 90 (Meteoswiss and EMPA) from fixed to free format.

```
com_mod.f90
conv_mod.f90
hanna_mod.f90
interpol_mod.f90
par_mod.f90
```

- ECMWF ï GFS
- No documentation folder
- Several bug corrections (check website, specially on dynamic allocation and overflows)

- Fortran 77 + some introduced Fortran 90 features

```
includecom
includeconv
includehanna
includeinterpol
includepar
```

- ECMWF ï GFS
- No documentation folder
- Several bug corrections (check website)

PLANNED DEVELOPMENTS: specified at the end

Versions and FLEXPART evolution

ECMWF versions ï GFS versions

- INPUT data:
  - ï ECMWF (several resolutions)
  - ï Nested input data possible
- Parameters read in
  - ï 5 3-D fields: horizontal and vertical wind components, temperature and specific humidity
  - ï 2-D fields: sfc pressure, total cloud cover, 10 m hor. wind components, 2 m temperature and dew point temperature, large scale and convective precipitation, sensible heat flux, east/west and north/south surface stress, topography, land- sea-mask and subgrid standard deviation of topography
- (some) of the params. calculated
  - ï surface stress and sensible heat flux(if they are missing missing and using the profile method) and friction velocity

- INPUT data:
  - ï GFS (0.5 deg horizontal)
  - ï Nested input data NOT possible
- Parameters read in
  - ï 5 3-D fields: horizontal and vertical wind components, temperature and relative humidity (transformed to specific humidity)
  - ï 2-D fields: sfc pressure, total cloud cover, 10 m hor. wind components, 2 m temperature and dew point temperature, large scale and convective precipitation, topography, land-sea-mask and subgrid standard deviation of topography
- (some) of the params. Calculated
  - ï spec humidity, friction velocity and sshf and 2m dew point temperature
- **IMPORTANT**: GFS files do not have all the fields at all times! Total cloud cover is not always present (this needs to be addressed by the user)

FLEXWRF v 2.1 (J. Brioude - NOAA)

Basic technical aspects

- Based on PILT (or flexpart-wrf 6.2 --- Fast and Easter 2006) but in Fortran 90 and with several differences
- The source code includes:
  - ï Serial version
  - ï OpenMP Ÿ multi-thread
  - ï Hybrid Parallel version MPI ï OpenMP Ÿ multi-core multi-thread
- There is no need of pre-processing the meteorological files. It directly reads WRF NESTED output in netCDF format Ÿ compilation with netCDF libraries

FLEXWRF v 2.1 (J. Brioude - NOAA)

Basic structural/file aspects

- The independent input files disappear and get merged into a UNIQUE input file ï `flexwrf.input` (following structure of WRF, for instance).

```
====================FORMER PATHNAMES FILE====================
/scratch2/portfolios/BMC/stela/jbrioude/flexout/
/scratch2/portfolios/BMC/gomtrans/angevine/wrf_CA_R23/
/scratch2/portfolios/BMC/calnexfc/angevine/flexpart/run/AVAILABLE3
=============================================================
====================FORMER COMMAND FILE=====================
     1                LDIRECT:          1 for forward simulation, -1 for backward
simulation
    20100503 040000  YYYYMMDD HHMISS   beginning date of simulation
    20100601 000000  YYYYMMDD HHMISS   end date of simulation
    3600             SSSSS             output every SSSSS seconds
    3600             SSSSS             time average of output (in SSSSS seconds)
    180              SSSSS             sampling rate of output (in SSSSS seconds)
    999999999        SSSSS             time constant for particle splitting (in seconds)
    180              SSSSS             synchronisation interval of flexpart (in seconds)

...........
```

FLEXWRF v 2.1 (J. Brioude - NOAA)

Basic structural/file aspects

- The AVAILABLE file changes in structure (also the naming, AVAILABLE, AVAILABLE.grid2,...)

```
<blankline>
<blankline>
<blankline>
20110310 120000 'wrfout_d03_2011-03-10_12:00:00' ''
20110310 130000 'wrfout_d03_2011-03-10_13:00:00' ''
20110310 140000 'wrfout_d03_2011-03-10_14:00:00' ''
20110310 150000 'wrfout_d03_2011-03-10_15:00:00' ''
20110310 160000 'wrfout_d03_2011-03-10_16:00:00' ''
20110310 170000 'wrfout_d03_2011-03-10_17:00:00' ''
```

Versions and FLEXPART evolution

FLEXWRF v 2.1 (J. Brioude - NOAA)

http://www.progonos.com/furuti/MapProj/Normal/ProjCon/projCon.html

Numerics, physics and new options

- Computational grid is the WRF [projected] native one.
- Output on an X-Y grid on the projected map (_reg routines)
- Output files are generated into the FLEXPART binary format (also ASCII version)
- Mesoscale fluctuations (meandering) ARE NOT switched off (as opposite to PILT ï check for instance the work of Belusic and Güttler, 2010 ñCan mesoscale models reproduce meandering?ò
- Turbulence scheme ï One may choose whether use the default FLEXPART scheme (recommended) or one based on the TKE fields from the WRF runs
- Possibility to use instantaneous omega (sigmadot), time-averaged wind, the usual instantaneous Cartesian vertical velocity calculated in FLEXPART that is based on mass continuity ï recommended the first (Brioude et al. 2012, GMD)

Versions and FLEXPART evolution

FLEXWRF v 2.1 (J. Brioude - NOAA)

- Map factors due to projection are included (were not in PILT)
- Modification of the pbl_profile to avoid problems with the von Kármán constant
- Deposition kernel modified so that the first three hours of a lifetime of a particle it is not used (preventing from smoothing close to the source)
- Wet and dry deposition implemented ï Wet deposition modified so that it does not depend on the cloud cover but whether a cloud is diagnosed or not. Subgrid scale variability erased
- Added the reading of parameters for the aerosols (bug in the calculation of cunningham ï Jerome check, please, `readinput.f90`, `part0.f90` had `cun` variable missing)
- Several bug fixes (see documentation when version is released)

FLEXWRF v 2.1 (J. Brioude - NOAA)

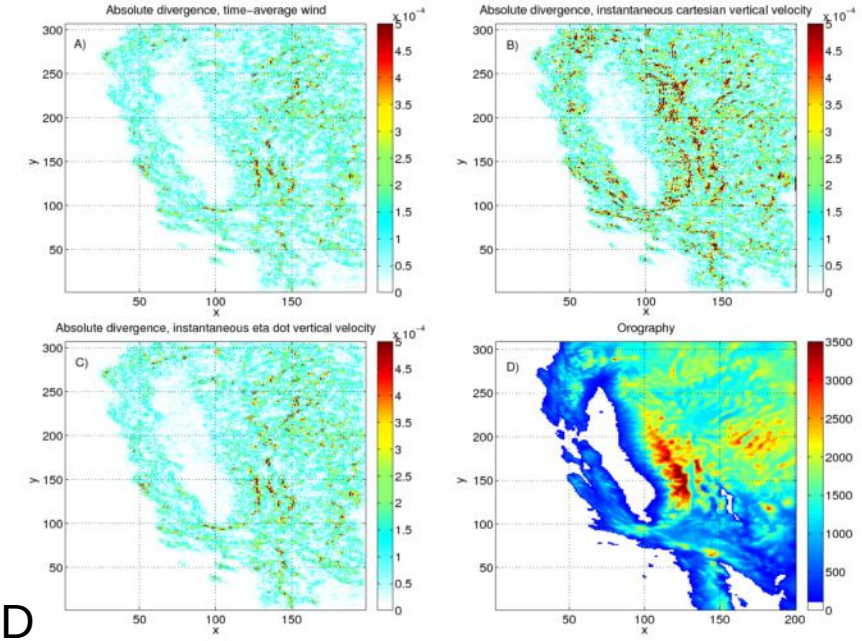
Further development

- Modification of the wet deposition scheme to activate sub.grid scale variability for a WRF-nested configuration with coarse resolution in the outermost domain
- Testing of the convecting scheme
- Improve the PBL scheme. add simple chemistry using output from WRF-Chem.

FLEXWRF v 2.1 (J. Brioude - NOAA)

WRF requirements

- Output the cloud fraction (optional ï currently not used)
- Ensure the registry has 'AVGFLX_RUM' , 'AVGFLX_RVM' , 'AVGFLX_WWM' and a BL parameterization that outputs the TKE depending on options wanted.
- Remember first WRF output file is 00 ï nothing really calculated and only interpolation... start with the actual first forecast time



Brioude et al. 2012 GMD

Fig. 1. Absolute wind divergence at about 50 m in altitude using **(a)** time-average wind, **(b)** instantaneous wind with cartesian vertical velocity, and **(c)** instantaneous wind with sigma dot (in s^{-1}). **(d)** Orography (in m).

Versions and FLEXPART evolution

FLEXPARTv8- COSMO https://wiki.c2sm.ethz.ch/Wiki/DocFlexpart

- ECMWF on a regular latitude-longitude grid, COSMO on a rotated latitude-longitude grid.
- ECMWF terrain following hybrid-pressure, COSMO a terrain-following hybrid-Z system.
- FLEXPART terrain-following Cartesian coordinate system. In the COSMO-FLEXPART version all fields are preserved on the original hybrid-Z grid.
- FLEXPART first converts the ECMWF omega field (Pa/s) to vertical wind (m/s) (covariant velocity) which is then corrected for horizontal transport in a sloping terrain to derive the vertical wind relative to the topography (contravariant velocity). COSMO winds are provided in m/s and a similar conversion to the contravariant velocity is necessary.
- COSMO uses different GRIB code tables and outputs different variables than ECMWF.
- FLEXPART requires a landuse map. A corresponding map has to be generated for the COSMO domain.
- COSMO winds are defined on grid cell boundaries (Arakawa-C/Lorenz grid) whereas ECMWF winds are obtained for cell centres. In COSMO, U and V are provided in the rotated system while 10 m winds are given in geographical (non-rotated) coordinates

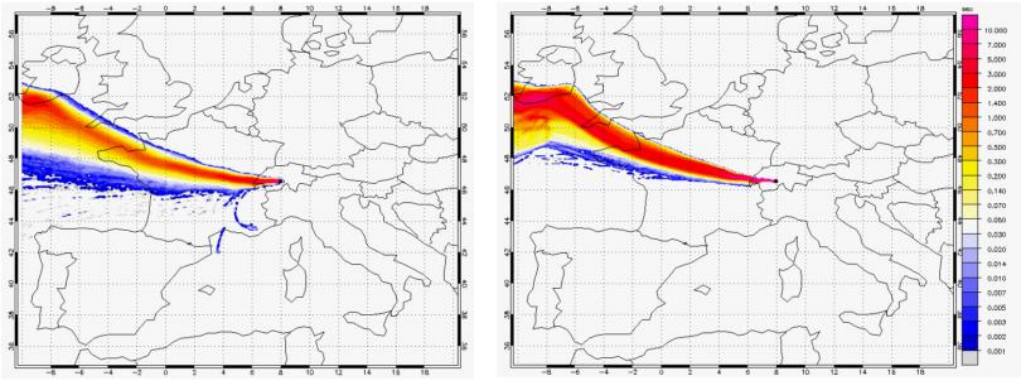
Versions and FLEXPART evolution

FLEXPARTv8- COSMO https://wiki.c2sm.ethz.ch/Wiki/DocFlexpart

Situation with strong westerly flow, 23 Jan 2009

Residence time maps 0-500 m above ground [s]

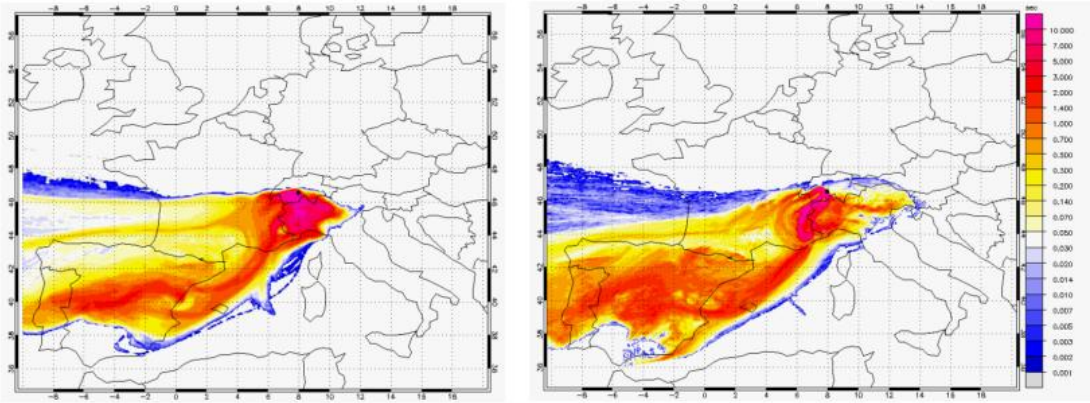
ECMWF **COSMO-7**



South Föhn event, 20 Jan 2009

Residence time maps 0-500 m above ground [s]

ECMWF **COSMO-7**



Versions and FLEXPART evolution

Developers workshop 2012

- Introduction of decay chains
- Optional new treatment of convection (skewed turbulence) from Cassini
- Dust emission pre-processing system and a plume-rise model
- Possibility to output wet+dry, wet and dry.
- Termination of runs after certain mass threshold is reached
- Improvements in the deaccumulation of precip and fluxes from ECMWF to avoid smoothing
- Re-evaluation of washout coefficients
- Adaptative output grid
- Otuput optional in netCDF
- Better error messages
- Namelists with default parameters
- TESTBED - Introduction of testdata and benchmarks in the main website