EXERCISE 1
Forward “Hello World” example

Aims:

1. Familiarise with FLEXPART structure and output
2. Set-up and execute a simple scenario
3. Plotting the output
4. Effect of the OUTGRID resolution
5. Effect of the number of particles

Questions? Write delia.arnold-arias@zamg.ac.at

Compiling FLEXPART on ZAMG’s virtual machines

```
#ifeq ($(gcc), 4.9)
# Compiled libraries under user ~flexpart, gfortran v4.9
#       ROOT_DIR = /homevip/flexpart/

#       F90       = ${ROOT_DIR}/gcc-4.9.1/bin/gfortran
#       MPIF90    = ${ROOT_DIR}/bin/mpifort

#       INCPATH1  = ${ROOT_DIR}/gcc-4.9.1/include
#       INCPATH2  = ${ROOT_DIR}/include
#       LIBPATH1 = ${ROOT_DIR}/lib


        #  System libraries at ZAMG, gfortran 4.9.2
        F90       = gfortran
        MPIF90    = mpif90

        INCPATH1 = $(GRIB_API_INCDIR)
        INCPATH2 = $(NETCDF_INCDIR)
        LIBPATH1 = $(GRIB_API_LIBDIR)
        LIBPATH2 = $(NETCDF_LIBDIR)

#else
# Compiled libraries under user ~flexpart, gfortran v5.4
#       ROOT_DIR = /homevip/flexpart/

#       F90       = /usr/bin/gfortran
#       MPIF90    = /usr/bin/mpifort

#       INCPATH1  = ${ROOT_DIR}/gcc-5.4.0/include
#       INCPATH2  = /usr/include
#       LIBPATH1 = ${ROOT_DIR}/gcc-5.4.0/lib
#endif
```

- tar -xvf flexpart_v10.3.1_3cd0f17.tar
- Edit makefile (see box to the left)
- Compile: **make serial**

- For compilation in parallel mode with MPI see Pisso et al., 2019. in GMD.

Edit par_mod.f90 (for ECMWF data):

- integer,parameter :: nxmax=800,nymax=400,nuvzmax=138,nwzmax=138,nzmax=138, nxshift=0
- integer,parameter :: maxnests=1,nxmaxn=800,nymaxn=400
- integer,parameter :: maxpart=5000000
- integer,parameter :: maxspec=10

```
LIBS = -lgrib_api_f90 -lgrib_api -lm -lnetcdff
LDFLAGS  = $(FFLAGS) -L$(LIBPATH1) -Wl,-rpath,$(LIBPATH1) $(LIBS) -L$(LIBPATH2)
LDDEBUG  = $(DBGFLAGS) -L$(LIBPATH1) $(LIBS) -L$(LIBPATH2)
```

Some preparations… Preparing the structure

1. **mkdir exercises** → make the *exercises* folder

2. **cd exercises** → enter the *exercises* folder

3. **mkdir Hello_World_fwd** and **cd Hello_World_fwd** → make the directory for your hello world forward exercise

4. **ln -s /path/to/metdata/ECMWF_meteorological_input/ ./** or **ln -s /path/to/metdata/NCEP_meteorological_input/ ./**

Find the necessary meteorological input data sets in "ECMWF_meteorological_input" and "NCEP_meteorological_input" for all the hands-on which path has to be entered in the respective pathnames file later on.
Meteorological files are heavy and it is best not to copy them in multiple places, linking is ideal.

Some preparations… Preparing the structure

1. **mkdir exercises** → make the *exercises* folder

2. **cd exercises** → enter the *exercises* folder

3. **mkdir Hello_World_fwd** and **cd Hello_World_fwd**

4. **ln -s /path/to/metdata/ECMWF_meteorological_input/ ./** or **ln -s /path/to/metdata/NCEP_meteorological_input/ ./**

5. Copy pathnames file and options folder from FLEXPART 10 folder. Pathnames file has to be edited accordingly for every exercise!

6. **cd options** Replace sub-folder SPECIES by ln -s /path/to/SPECIES/ ./

7. Link FLEXPART gfortran executable to working directory (i.e., Hello_World_fwd)

8. cp /path/to/plotting/plot_FLEX_binary.py ./
   cp /path/to/plotting/read_header.py ./
   cp /path/to/plotting/read_grid.py ./

9. mkdir output_[ECMWF,NCEP]

Remember steps 3 to 9 for all test cases!

Hello World fwd & plotting

This test case aims at making you run FLEXPART with a very simple case to warm-up for the following, more complicated FLEXPART options

Specifications:

- COMMAND FILE:
  - Forward run: 1 March 2007 9 am UTC to 2 March 2007 14 UTC
  - Output every hour
  - Convection
  - Concentration output
  - Nested output
  - No adaptation to TL
- OUTGRID FILE:
  - Resolution 0.1 degree
  - LLC: 37.0° N, 0.0° E
  - 70 x 200 grid cells
  - 1 output layer, 250 m a.g.l.

Launch FLEXPART!

- OUTGRID NEST
  - Resolution 0.015
  - 420 x 220 grid cells
  - LLC 37.5° N° E. 1.0° E
- RELEASES FILE:
  - Point source at the top of the INTE building: 41.384° N, 2.116° E, 60 m a.g.l.
  - Release start: 1 March 2007 9 UTC
  - Release end: 1 March 2007 21 UTC
  - Total mass: 21 kg of SO4 aerosol
  - Particles released: 10000

Does all this make sense? What does this mean? Discuss results and test different output resolutions. The sync and average times. Number of particles.

Hello World fwd & plotting

- **Reflexible (evolution of pflexible)** John Burkhart
  https://github.com/spectraphilic/reflexible

+ Python based

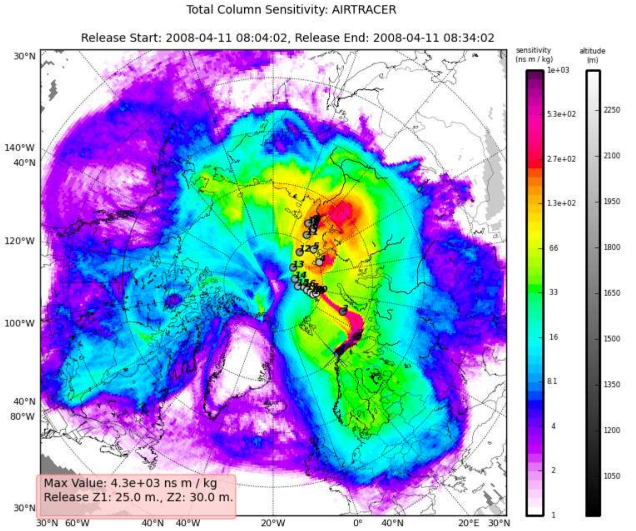
+ handle both binary and netcdf output

+ Easy folding with gridded inventories

+ ZAMG uses a variation of it operationally

+ Additional routines for dumping information and processing files (accumulate)

+ Simple plotting and complex plotting



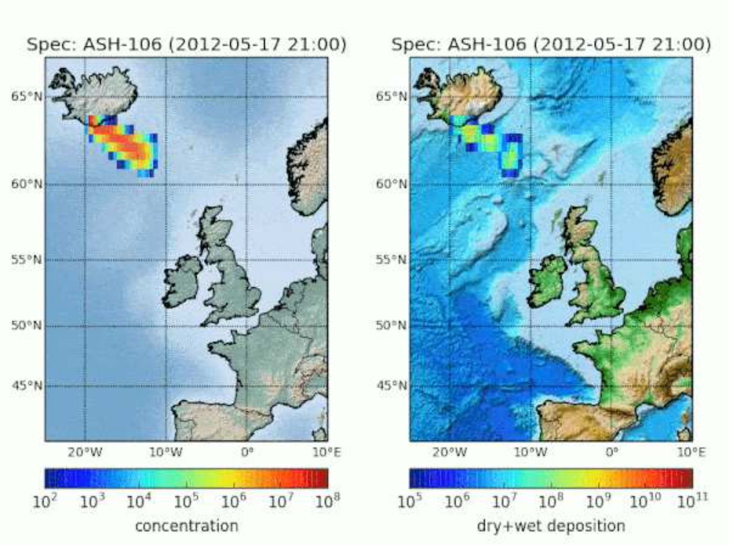
- **QuickLook** Radek Hofman https://bitbucket.org/radekhofman/quicklook/

  - Based on flex_81.py
  - Under development

+ Easy command line parameters

+ Responsive developer

+ Python based



Hello World fwd & plotting

Even some options for 3D plotting

- **Matlab**: - Requires license
  - Not fast

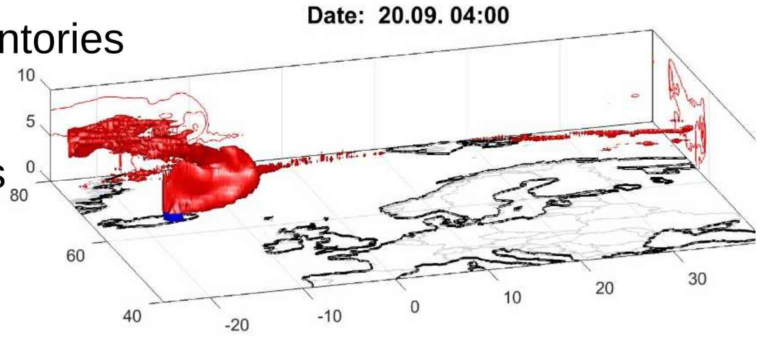
Sabine Eckhardt (NILU)

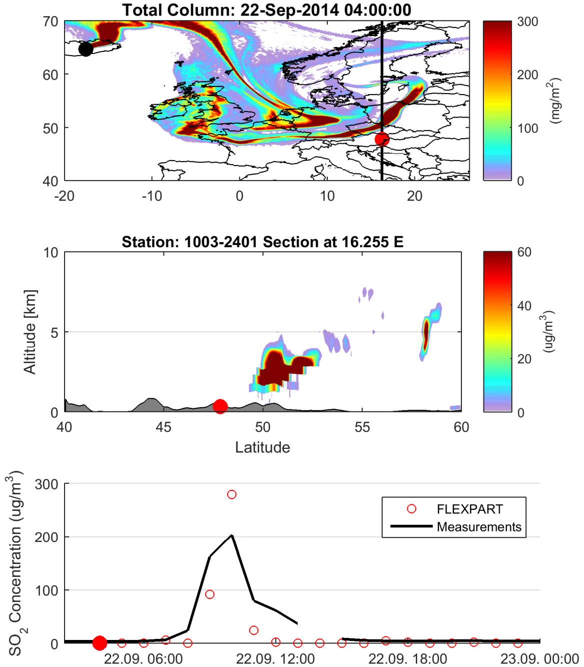
+ Easy folding with gridded inventories

+ nice 3D plotting capabilities

+ designed to deal with matrices

+ rendering possible





- **`plot_FLEX_binary.py`**

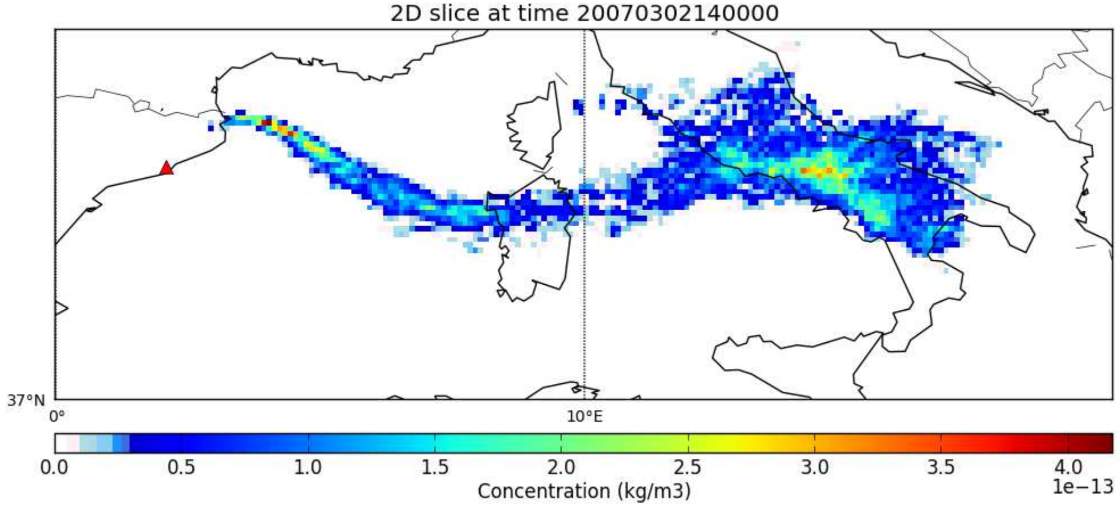
Delia Arnold (ASC, ZAMG), Christian Maurer (ZAMG), Don Morton (Boreal SciCom)

+ Free

+ Simple to use

+ Python based

- Very limited and developed for in-house use or testing



Hello World fwd & plotting

Note there is the option of plotting the NetCDF output

- https://www.giss.nasa.gov/tools/panoply/download/ PANOPLY(useful for Windows users)
- http://meteora.ucsd.edu/~pierce/ncview_home_page.html NCVIEW
- …

ECMWF: Hello World fwd & plotting

Results: Did you get a ‘congratulations’ message on your run?

- Yes → We should see the output produced
- No → Were the option files well set? Was the compilation appropriate for your run? Is recompilation (with adjustment of par_mod.f90) needed?

```
./plot_FLEX_binary.py ./output_ECMWF/ False tracer1 0 0 alldates cyl False
0,20,37,44 mesh False
```

Output directory

False – plot the MOTHER domain

Species name

Level index (0: first level)

Release index (0: first release)

Dates to plot: „alldates“ or user-defined list of dates, e.g., 20170925000000, 20170925010000

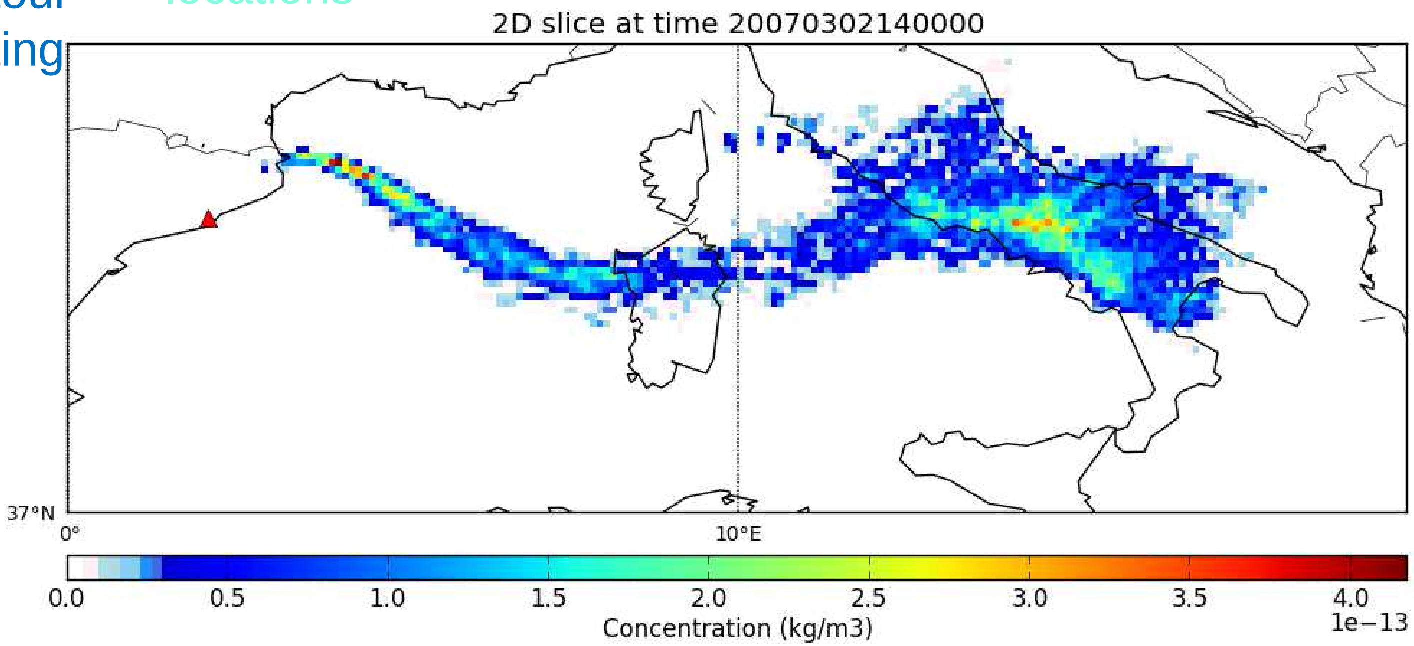
Projection : Lambert or cylindric

No deposition plotted

Plotting region: left and right lon, lower and upper lat

Mesh or contour plotting

Add marked locations

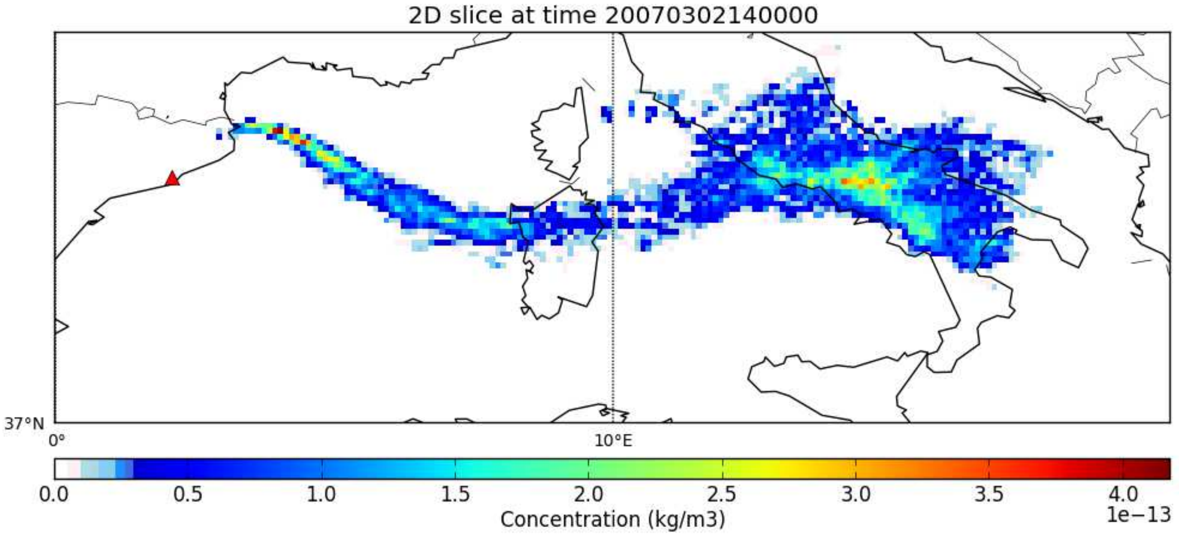


ECMWF: Hello World fwd & plotting

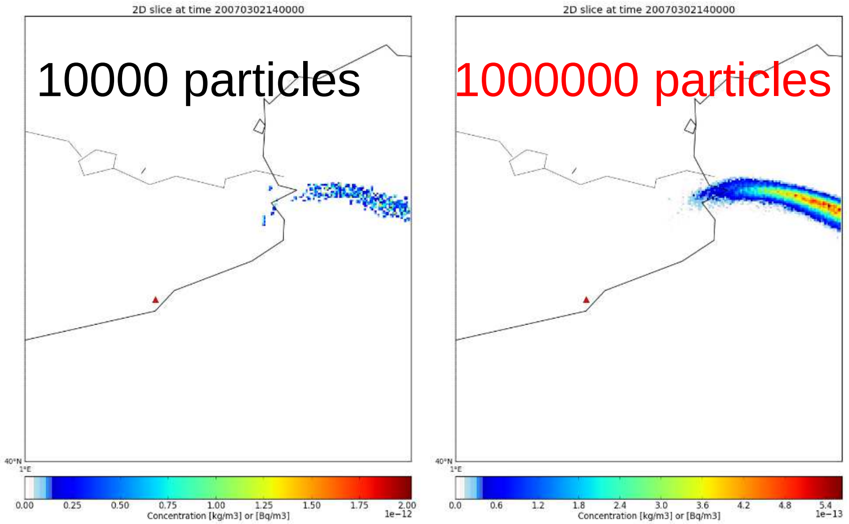
Results: Did you get a ‘congratulations’ message on your run?

- Yes → We should see the output produced
- No → Were the option files well set? Was the compilation appropriate for your run? Is recompilation (with adjustment of par_mod.f90) needed?

```
./plot_FLEX_binary.py ./output_ECMWF/ False 1 0 0 alldates cyl False
0,20,37,44 mesh False
./plot_FLEX_binary.py ./output_ECMWF/ True 1 0 0 alldates cyl True
1.0,4.3,40.0,43.8 mesh False
```



Effect of number of particles...

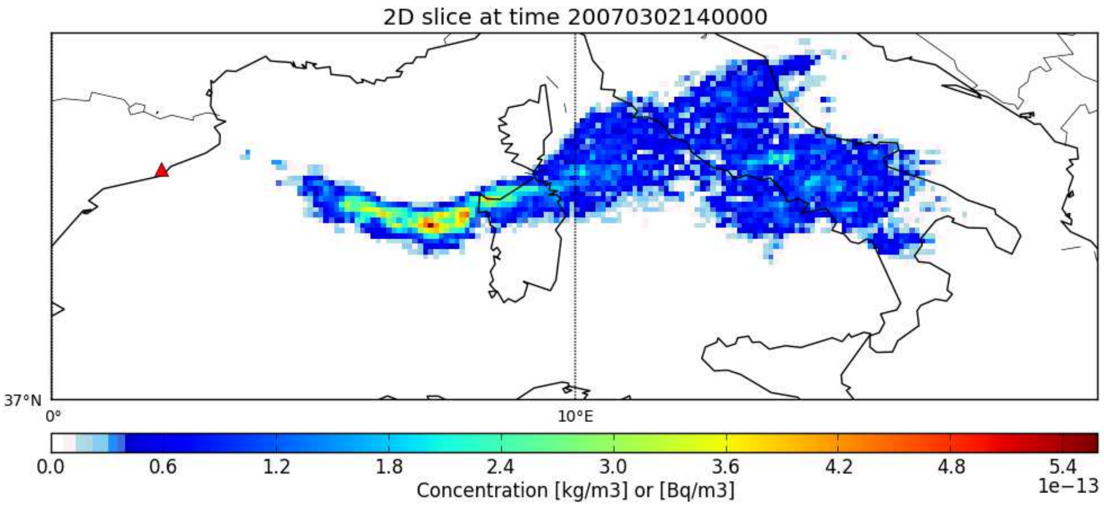

2D slice at time 20070302140000
10000 particles
40°N
1°E
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
1e−12
Concentration [kg/m3] or [Bq/m3]
2D slice at time 20070302140000
1000000 particles
40°N
1°E
0.0
0.6
1.2
1.8
2.4
3.0
3.6
4.2
4.8
5.4
1e−13
Concentration [kg/m3] or [Bq/m3]

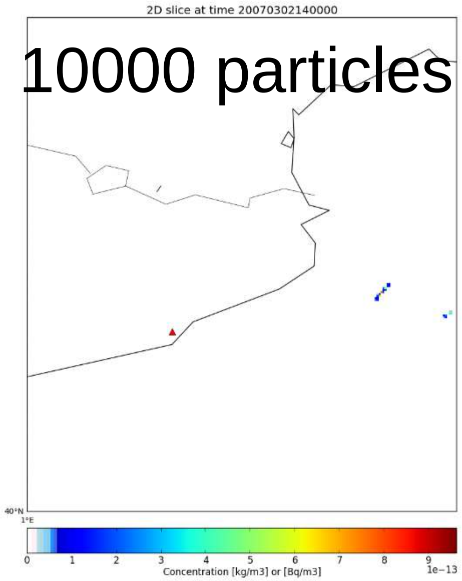
NCEP: Hello World fwd & plotting

Results: Did you get a ‘congratulations’ message on your run?

- Yes → we should see the output produced
- No → where the option files well set? Was the compilation appropriate for your run? Is recompilation (with adjustment of par_mod.f90) needed?

```
./plot_FLEX_binary.py ./output_NCEP/ False 1 0 0 alldates cyl False
0,20,37,44 mesh False
./plot_FLEX_binary.py ./output_NCEP/ True 1 0 0 alldates cyl True
1.0,4.3,40.0,43.8 mesh False
```


2D slice at time 20070302140000
37°N
0°
10°E
0.0
0.6
1.2
1.8
2.4
3.0
3.6
4.2
4.8
5.4
1e−13
Concentration [kg/m3] or [Bq/m3]

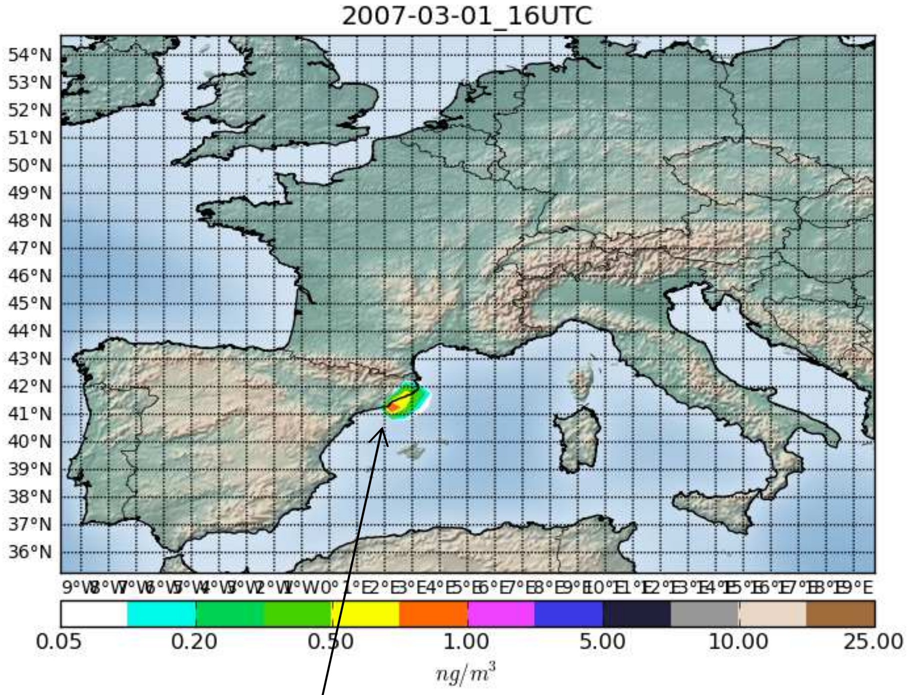

10000 particles

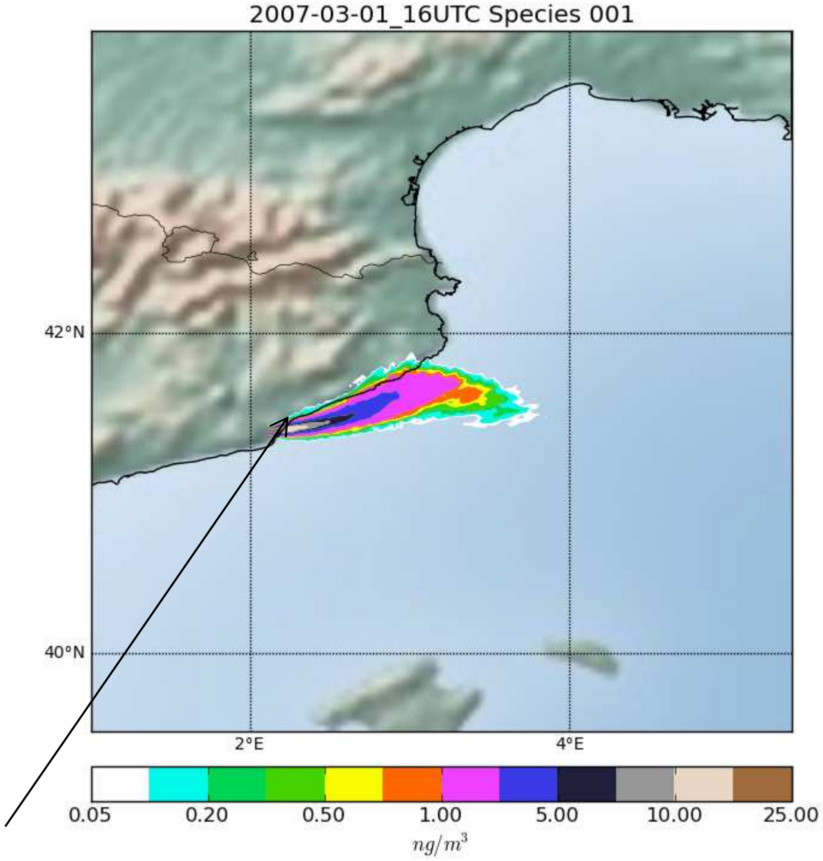
2D slice at time 20070302140000
40°N
1°E
0
1
2
3
4
5
6
7
8
9
1e−13
Concentration [kg/m3] or [Bq/m3]

Hello World fwd & plotting

Results: plots of concentrations

What can we see?

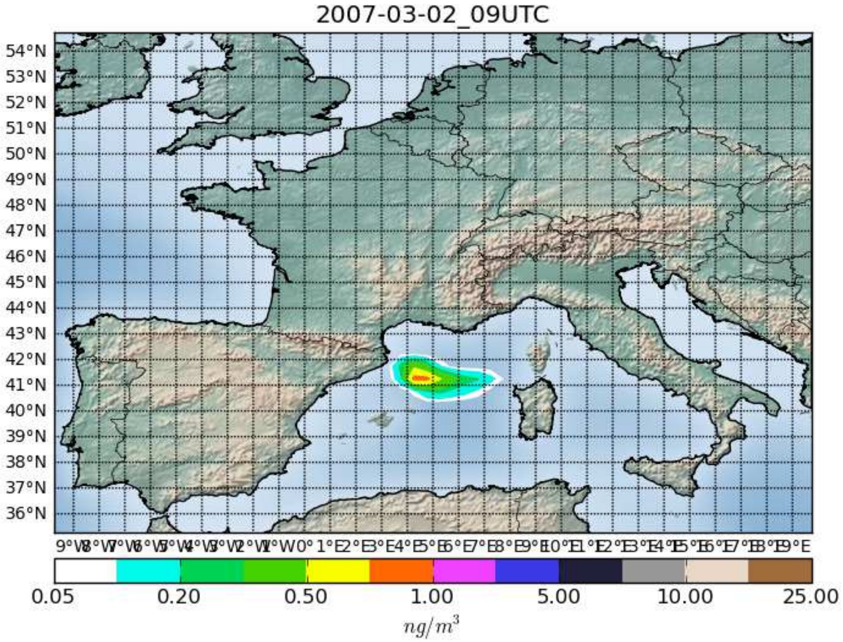


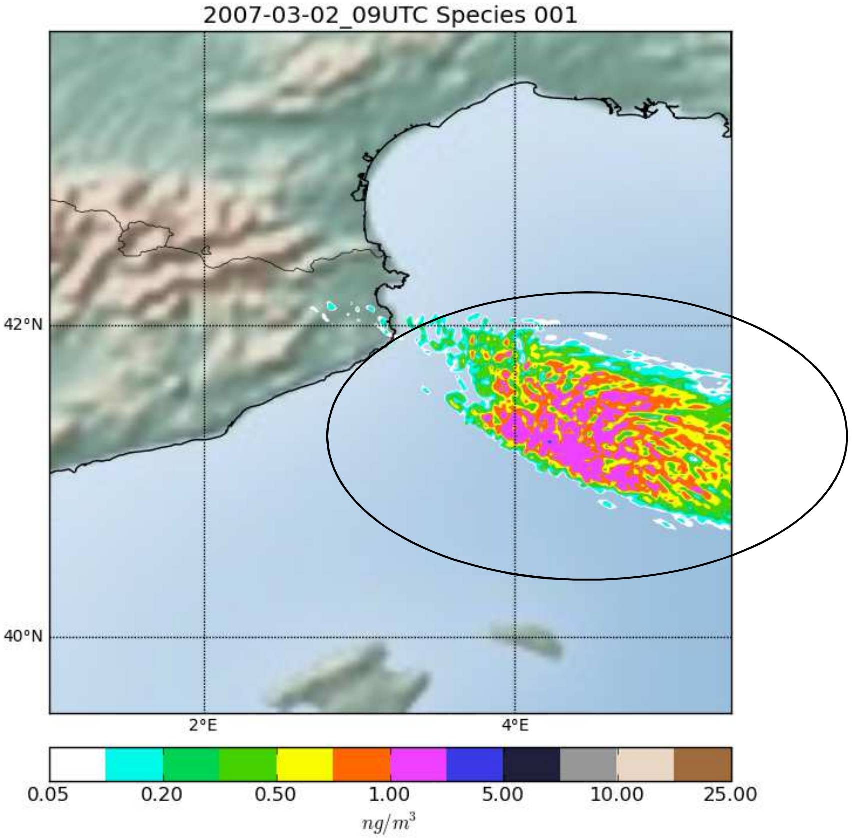


Effect of OUTGRID resolution: Sharper and larger maxima, less smooth edges…

Hello World fwd & plotting

Results: *What can we see?*

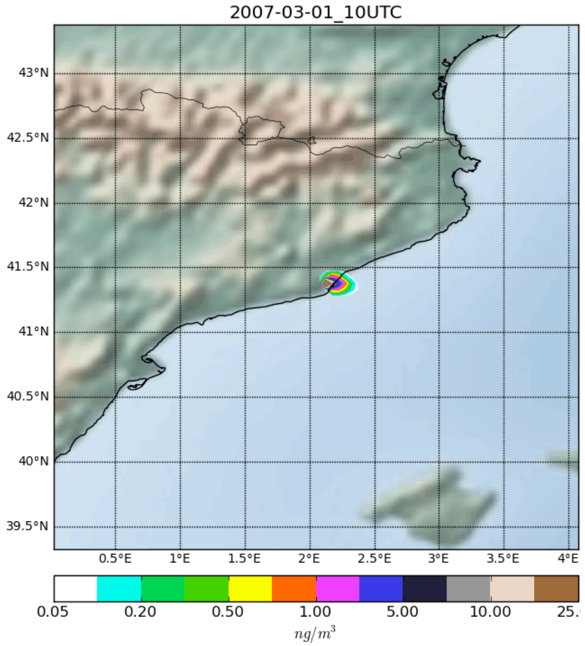


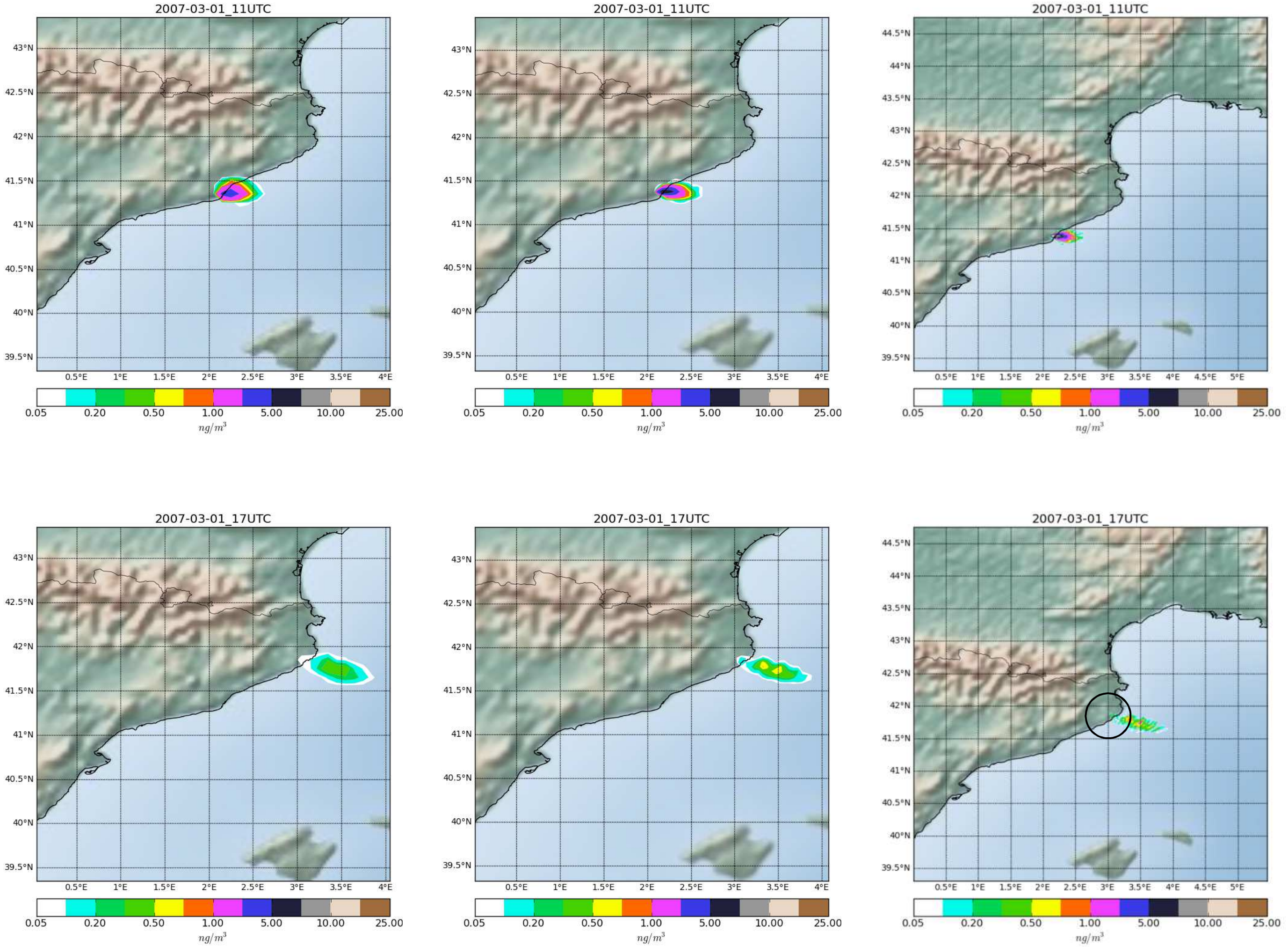


Effect of number of particles...

Hello World fwd & plotting

Another example: Output1 – 0.1 - 0.05 - 0.015





What does happen when resolution increases while keeping the number of particles ?

Hello World fwd & plotting

What to do?

Options:

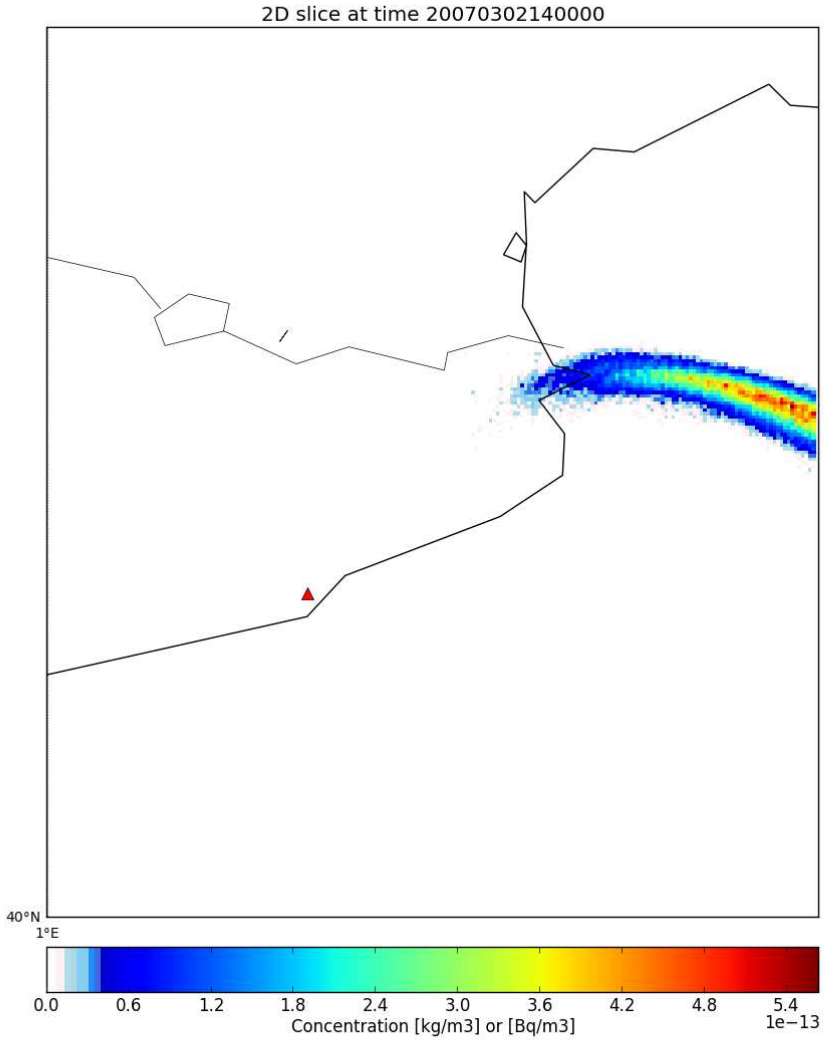
- Increase the number of particles → larger computational demands (FLEXPART 10 & FLEXPART-WRF are parallel/have option for a parallel executable) and the problem may appear later
- Particle splitting → it increases the particles after a user-defined time-step. Number of particles increases exponentially and so do the computational times
- Larger grid sizes (horizontal and vertical) so that more particles are sampled → smoothing

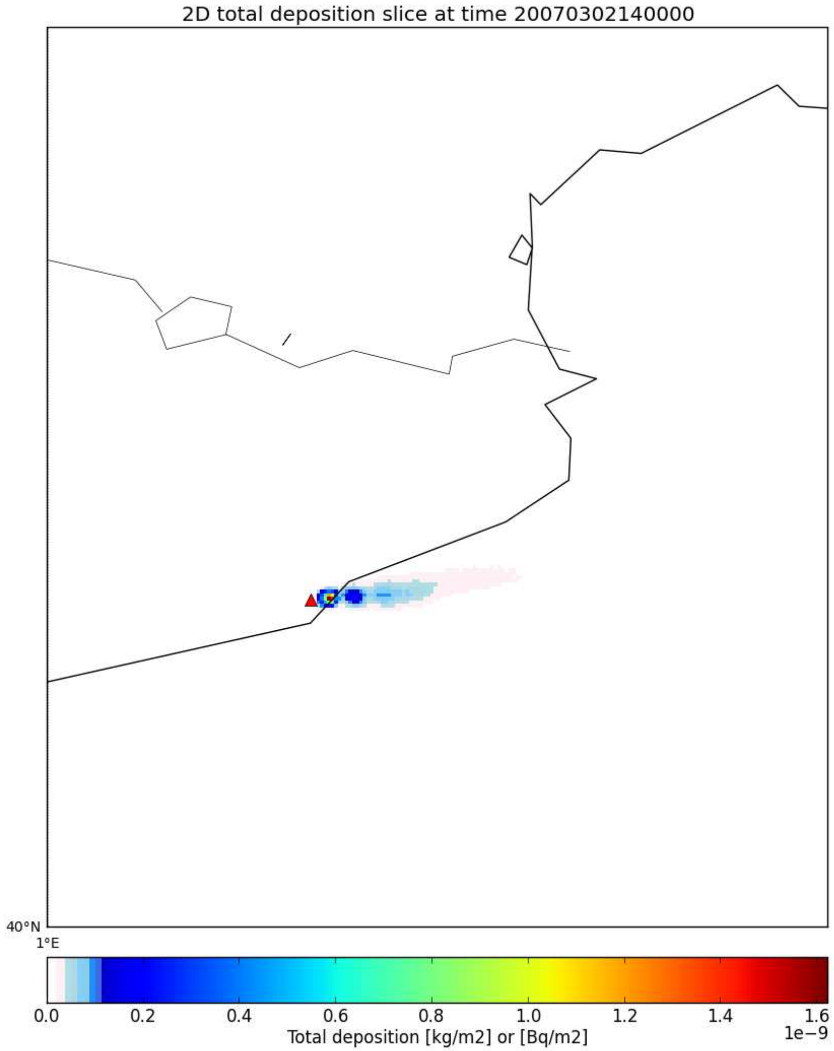
- No perfect solution, **trade-offs** need to be made

ECMWF: Hello World fwd & plotting

Results: Concentration and deposition

What can we see?


2D slice at time 20070302140000


2D total deposition slice at time 20070302140000