FLEXPART training course 2013: structure

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L2

FLEXPART structure

Meteo input

AVAILABLE
EN200701010000
...

Use appropriate tree structure

Options

COMMAND
OUTGRID , _NEST
RELEASES
RECEPTORS
AGECLASSES
*.t

pathnames makefile

FLEXPART

Includecom / com_mod.f90
includepar / param_mod.f90
include* / *mod.f90
*.f / *.f90

output

grid_conc_YYYYMMDDHHMMSS_SSS
grid_time_YYYYMMDDHHMMSS_SSS
grid_pptv_YYYYMMDDHHMMSS_SSS
partposit_date
trajectories.txt

SPECIES

SPECIES_001
SPECIES_002
…

SPECIES_XXX (user defined)

```
srvx7.img.univie.ac.at{/home/srvx7/flexpartcourse/DeliaTemp/Testcases/HelloWorld}91 %ls -lt
total 60
lrwxrwxrwx. 1 delia tmc   49 Apr  9 11:02 FLEXPART_ECMWF_GFORTRAN -> ../../../FLEXPART_PROGRAM
/FLEXPART_ECMWF_GFORTRAN
drwxrwxr-x. 3 delia tmc 4096 Apr  8 14:55 Output1
drwxrwxr-x. 3 delia tmc 4096 Apr  8 14:54 Output3
-rw-r--r--. 1 delia tmc  120 Apr  8 14:54 pathnames~
drwxrwxr-x. 3 delia tmc 4096 Apr  8 14:54 Options
drwxr-xr-x. 3 delia tmc 4096 Apr  8 14:53 Output
drwxrwxr-x. 3 delia tmc 4096 Apr  8 14:53 Output2
-rw-r--r--. 1 delia tmc  119 Apr  8 14:53 pathnames
srvx7.img.univie.ac.at{/home/srvx7/flexpartcourse/DeliaTemp/Testcases/HelloWorld}92 %
```

FLEXPART important files

pathnames

- Where all the files are and output should be kept. Formatting is strict! Beware, specially with the "/" at the end of the lines.

```
/home/as/FLEXPART50/options/
/volc/as/contrace/modelresults/forward/
/volc/windcontrace/
/volc/windcontrace/AVAILABLE
/volc/nested/
/volc/nested/AVAILABLE
==========================================

Line 1: path where control files "COMMAND" and "RELEASES" are available
Line 2: name of directory where output files are generated
Line 3: path where meteorological fields are available (mother grid)
Line 4: full filename of "AVAILABLE"-file (mother grid)

Subsequent lines:
Line 2n+3: path where meteorological fields are available (nested grid n)
Line 2n+4: full filename of "AVAILABLE"-file (nested grid n)

Line below last pathname must be:
==========================================

The grids must be arranged such as that the coarse-scale nests
come before the fine-scale nests. Multiple nests of the same
nesting level are allowed. In that case, the order is arbitrary.
```

With increasing resolution (up to 7 nests)

FLEXPART important files

Includepar (or param_mod.f90)

- It includes all the definition and setting of parameters. Important ones for the user: hmixmin, idiffnorm, maxpart, maxspec, ncluster

```
*******************************************************************************
      implicit none
*************************************************************
C Number of directories/files used for FLEXPART input/output
*************************************************************
      integer numpath
      parameter(numpath=4)
C numpath               Number of different pathnames for input/output files
******************************
C Physical and other constants
******************************
      real pi,pi180,r_air,r_earth,ga,cpa,kappa,vonkarman
      parameter(pi=3.14159265,r_earth=6.371e6,r_air=287.05,ga=9.81)
      parameter(cpa=1004.6,kappa=0.286,pi180=pi/180.,vonkarman=0.4)
C pi                    number "pi"
C pi180                   pi/180.
C r_earth                 radius of earth [m]
C r_air                  individual gas constant for dry air [J/kg/K]
C ga                     gravity acceleration of earth [m/s**2]
C cpa                     specific heat for dry air
C kappa                    exponent of formula for potential temperature
C vonkarman                 von Karman constant
      real karman,href,convke,hmixmin,hmixmax,turbmesoscale
      real d_trop,d_strat
      parameter(karman=0.40,href=15.,convke=2.0)
      parameter(hmixmin=100.,hmixmax=4500.,turbmesoscale=0.16)
      parameter(d_trop=50.,d_strat=0.1)
```

FLEXPART important files

COMMAND

- Basic runtime options, fwd bwd, time controls, init end date of SIMULATION (bwd or fwd) ...

```
*******************************************************************************
*                                                                             *
*      Input file for the Lagrangian particle dispersion model FLEXPART       *
*                           Please select your options                        *
*                                                                             *
*******************************************************************************

1. __                  3X, I2
    1
   LDIRECT             1 FOR FORWARD SIMULATION, -1 FOR BACKWARD SIMULATION

2. ________ ______     3X, I8, 1X, I6
   20040626 000000
   YYYYMMDD HHMISS     BEGINNING DATE OF SIMULATION

3. ________ ______     3X, I8, 1X, I6
   20040816 120000
   YYYYMMDD HHMISS     ENDING DATE OF SIMULATION

4. _____               3X, I5
    7200
   SSSSS               OUTPUT EVERY SSSSS SECONDS

5. _____               3X, I5
    7200
   SSSSS               TIME AVERAGE OF OUTPUT (IN SSSSS SECONDS)

6. _____               3X, I5
     900
```

FLEXPART important files

COMMAND

- All input files (for better generation of batch jobs) can be written in a compressed way (it reads free format):

```
 ++++++++++++ HEADER +++++++++++++++++
 ++++++++++++ HEADER +++++++++++++++++
 ++++++++++++ HEADER +++++++++++++++++
 ++++++++++++ HEADER +++++++++++++++++
 ++++++++++++ HEADER +++++++++++++++++
 ++++++++++++ HEADER +++++++++++++++++
 ++++++++++++ HEADER +++++++++++++++++
1
20040101 000000
20061231 210000
432000
432000
  900
 99999999
900   SYNC
-5.0  CTL
4     IFINE
1     IOUT
2     IPOUT
1     LSUBGRID
1     LCONVECTION
1     LAGESPECTRA
0     IPIN
0     IOFR
0     IFLUX
0     MDOMAINFILL
1     IND_SOURCE
1     IND_RECEPTOR
0     MQUASILAG
0     NESTED_OUTPUT
0     LINIT_COND      INITIAL COND. FOR BW RUNS: 0=NO,1=MASS UNIT,2=MASS MIXING RATIO UNIT
```

Output time: how often the output is printed out

Average time: averaged concentrations are averaged in this period

Sampling time: times when concentrations are sampled to get the averages (< average time)

Synchronisation time: internal time-step (all times multiple of this one)

FLEXPART important files

COMMAND

- All input files (for better generation of batch jobs) can be written in a compressed way:

```
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
1
20040101 000000
20061231 210000
432000
432000
  900
 99999999
900   SYNC
-5.0  CTL
4     IFINE
1     IOUT
2     IPOUT
1     LSUBGRID
1     LCONVECTION
1     LAGESPECTRA
0     IPIN
0     IOFR
0     IFLUX
0     MDOMAINFILL
1     IND_SOURCE
1     IND_RECEPTOR
0     MQUASILAG
0     NESTED_OUTPUT
0     LINIT_COND      INITIAL COND. FOR BW RUNS: 0=NO,1=MASS UNIT,2=MASS MIXING RATIO UNIT
```

CTL > 0 adaptation to Lagrangian time scales (recommended)

Type of output

Particle dump

Moist convection – computationally demanding

Tracking the releases independently (a must for backward runs)

FLEXPART important files

COMMAND

- All input files (for better generation of batch jobs) can be written in a compressed way:

```
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
+++++++++++++ HEADER +++++++++++++++++
1
20040101 000000
20061231 210000
432000
432000
   900
 99999999
900   SYNC
-5.0  CTL
4     IFINE
1     IOUT
2     IPOUT
1     LSUBGRID
1     LCONVECTION
1     LAGESPECTRA
0     IPIN
0     IOFR
0     IFLUX
0     MDOMAINFILL
1     IND_SOURCE
1     IND_RECEPTOR
0     MQUASILAG
0     NESTED_OUTPUT
0     LINIT_COND      INITIAL COND. FOR BW RUNS: 0=NO,1=MASS UNIT,2=MASS MIXING RATIO UNIT
```

→ Age spectra: to separate concentrations according to „age“ and also to give a finite life to a single species particle

FLEXPART important files

RELEASES

- Set the number of releases, shape, species released, temporal variations if needed – same for fwd and bwd!

```
*****************************************************************************
*                                                                           *
*                                                                           *
*                                                                           *
*   Input file for the Lagrangian particle dispersion model FLEXPART        *
*                         Please select your options                        *
*                                                                           *
*                                                                           *
*                                                                           *
*****************************************************************************
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
  1
___                        i3    Total number of species emitted

 24
___                        i3    Index of species in file SPECIES

=============================================================================
20011028  150007
________ ______            i8,1x,i6 Beginning date and time of release

20011028  150046
________ ______            i8,1x,i6 Ending date and time of release

   9.4048
____.____                  f9.4  Longitude [DEG] of lower left corner

  48.5060
____.____                  f9.4  Latitude [DEG] of lower left corner
```

Header

Basic info: number of species and their ideces successively

All particles will carry the species, mass for each should be set in each release

FLEXPART important files

RELEASES

- Set the number of releases, shape, species released, temporal variations if needed – same for fwd and bwd!

```
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++ HEADER ++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++++++++
      2
    201
    202

  20040101      0
  20040131   240000
 29.00000
 59.00000
 30.00000
 60.00000
      1
   0.0000
 100.0000
 500000
 179724.7
 179724.7
STPBRG01020101
```

→ Interval of release

→ Location of the release

→ m a.g.l (1) m a.s.l (2) hPa pressure (3)

→ m a.g.l (1) m a.s.l (2) hPa pressure (3)

→ Number of particles

→ Mass carried for the particles of each species

FLEXPART important files

OUTGRID / OUTGRID_NEST

- Description of the domain where the concentrations, residence times... will be output

It is useful to make the nest fit within full mother grid cells (e.g. if folding with an emission inventory is made a posteriori)

```
*******************************************************************************
*                                                                             *
*     Input file for the Lagrangian particle dispersion model FLEXPART        *
*                     Please specify your output grid                         *
*                                                                             *
*******************************************************************************

1.  ------.----       4X,F11.4
     -179.0000       GEOGRAFICAL LONGITUDE OF LOWER LEFT CORNER OF OUTPUT GRID
    OUTLONLEFT       (left boundary of the first grid cell - not its centre)

2.  ------.----       4X,F11.4
      -90.0000       GEOGRAFICAL LATITUDE OF LOWER LEFT CORNER OF OUTPUT GRID
    OUTLATLOWER      (lower boundary of the first grid cell - not its centre)

3.  -----             4X,I5
     360              NUMBER OF GRID POINTS IN X DIRECTION (= No. of cells + 1)
    NUMXGRID

4.  -----             4X,I5
     180              NUMBER OF GRID POINTS IN Y DIRECTION (= No. of cells + 1)
    NUMYGRID

5.  ------.---        4X,F10.3
        1.000        GRID DISTANCE IN X DIRECTION
    DXOUTLON

6.  ------.---        4X,F10.3
        1.000        GRID DISTANCE IN Y DIRECTION
    DYOUTLAT

10. -----.-           4X, F7.1
      100.0
    LEVEL 4          HEIGHT OF LEVEL (UPPER BOUNDARY)

10. -----.-           4X, F7.1
     3000.0
    LEVEL 4          HEIGHT OF LEVEL (UPPER BOUNDARY)
```

FLEXPART important files

OUTGRID / OUTGRID_NEST

```
*******************************************************************************
*                                                                             *
*     Input file for the Lagrangian particle dispersion model FLEXPART        *
*                     Please specify your output grid                         *
*                                                                             *
*******************************************************************************

1.  ------.----      4X,F11.4
      -15.0000      GEOGRAFICAL LONGITUDE OF LOWER LEFT CORNER OF OUTPUT GRID
    OUTLONLEFT      (left boundary of the first grid cell - not its centre)

2.  ------.----      4X,F11.4
       35.0000      GEOGRAFICAL LATITUDE OF LOWER LEFT CORNER OF OUTPUT GRID
    OUTLATLOWER     (lower boundary of the first grid cell - not its centre)

3.  -----            4X,I5
     220             NUMBER OF GRID POINTS IN X DIRECTION (= No. of cells + 1)
    NUMXGRID

4.  -----            4X,I5
     120             NUMBER OF GRID POINTS IN Y DIRECTION (= No. of cells + 1)
    NUMYGRID

5.  ------.-----     4X,F12.5
        0.25000      GRID DISTANCE IN X DIRECTION
    DXOUTLON

6.  ------.-----     4X,F12.5
        0.25000      GRID DISTANCE IN Y DIRECTION
    DYOUTLAT
```

No nesting in the vertical!

FLEXPART important files

RECEPTORS

- Locations where near ground concentrations (using the parabolic kernel) are to be given

```
*******************************************************************************
*                                                                             *
*     Input file for the Lagrangian particle dispersion model FLEXPART        *
*                     Please specify your receptor points                     *
*    For the receptor points, ground level concentrations are calculated      *
*                                                                             *
*******************************************************************************
1.  ----------------  4X,A16
   F15               NAME OF RECEPTOR POINT
   RECEPTORNAME

2.  ------.----       4X,F11.4
       6.1333       GEOGRAFICAL LONGITUDE
   XRECEPTOR

3.  ------.----       4X,F11.4
      49.0833       GEOGRAFICAL LATITUDE
   YRECEPTOR
===============================================================================
1.  ----------------  4X,A16
   NL01              NAME OF RECEPTOR POINT
   RECEPTORNAME

2.  ------.----       4X,F11.4
       5.7833       GEOGRAFICAL LONGITUDE
   XRECEPTOR

3.  ------.----       4X,F11.4
      50.9167       GEOGRAFICAL LATITUDE
   YRECEPTOR
===============================================================================
```

FLEXPART-WRF structure