Flex_extract v7.1: Extraction and preparation of ECMWF's meteorological data for the Lagrangian atmospheric transport model FLEXPART

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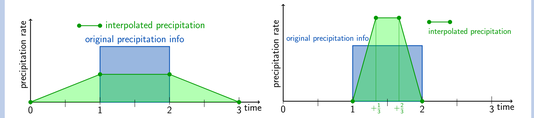
Introduction

The `flex_extract` Open-Source software package is a tool to extract and prepare meteorological data from the European Centre for Medium-Range Weather Forecasts (ECMWF) as input for the Lagrangian particle transport model FLEXPART ([1],[5],[6],[4]). These data fields describe the state of the atmosphere relevant for transport modelling. A special feature is the processing of parameterized vertical surface fluxes, which are only available as accumulated forecast values and therefore need to be deaccumulated, in order to get the quasi-instantaneous fluxes which FLEXPART requires.
This poster gives an overview of the new, refurbished version 7.1 and the overall aim to increase the quality of deposition fields calculated from FLEXPART. Since it is not yet officially released, it can currently be cloned from the dev branch of the GIT repository on `http://flexpart.eu` for testing purposes. An extensive online documentation is currently in process and will soon be available on the community website along with the software package .

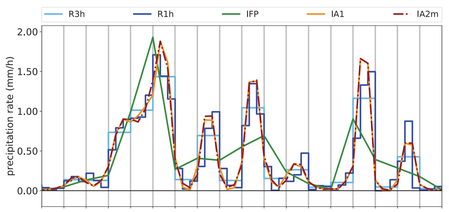
Schematic view of the precipitation disaggregation problem



left: old disaggregation method; right: new disaggregation method

New disaggregation method for precipitation

The reconstruction algorithm is based on a one-dimensional piecewise-linear function with two additional supporting points within each grid cell. The new method fulfils the desired requirements by preserving the integral precipitation in each time interval, guaranteeing continuity at interval boundaries, maintaining non-negativity, and being monotone.

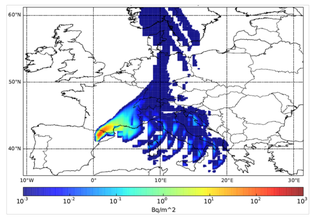


Short sequence from a convective precipitation time series. Raw precipitation curves from ECMWF are compared to the interpolated curves from `flex_extract`. For more information see [3].

- R3h 3-hourly precipitation from the ECMWF MARS archiv
- R1h 1-hourly precipitation from the ECMWF MARS archiv
- IFP Disaggregation and interpolation of 3 h precipitation to 1 h; using a modified, linear interpolation (old)
- IA1 Disaggregation and interpolation of 3 h precipitation to 1 h; non-negative, geometric mean based algorithm
- IA2m Modified IA1, UNUSED.

Overall aim to improve level of confidence in deposition

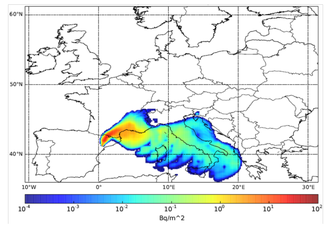
Before: deposition field with artifacts



Improvements in flex_extract:
- disaggregation scheme **(DONE, [3])**

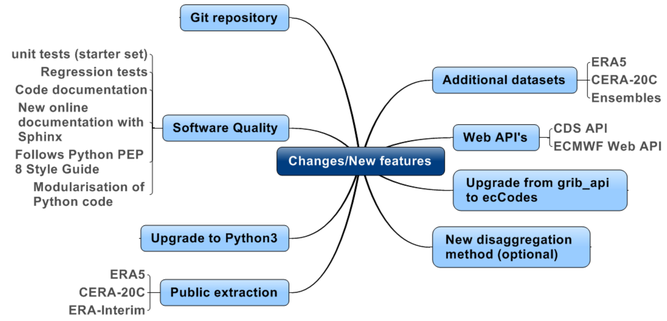
Improvements in FLEXPART:
- cloud diagnostics **(in progress)**
- Interpolation **(in progress)**
- Parameterization **(DONE, [2])**

Afterwards: reduced artifacts in the deposition field



Aim: e.g. Increase the quality of the deposition results

Changes and new features in `flex_extract v7.1`

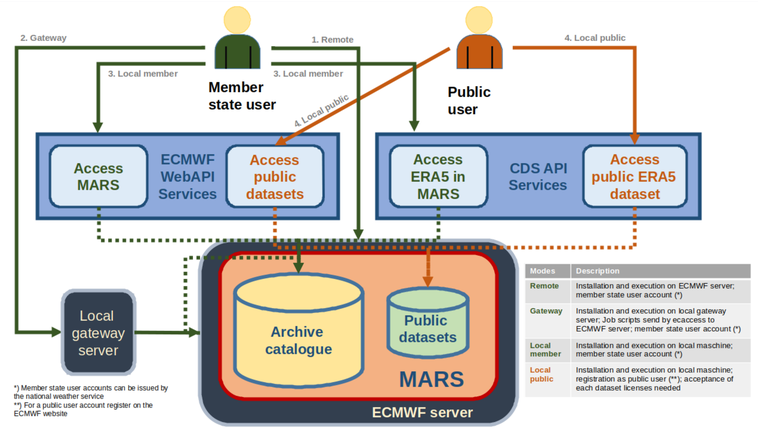


ECMWF data (available with `flex_extract`)

Differences in MARS parameters for the extraction of operational and various reanalysis data.
Member state user: Operational data, ERA-Interim, ERA5, CERA-20C
Public user: Re-analysis data sets ERA-Interim, ERA5, CERA-20C (partially limited)

	Operational	ERA-Interim	ERA5	CERA-20C
Period	12/1985 - ongoing	01/1979-12/2018	01/1979-12/2018	09/1901-12/2010
Streams	oper/elda/enfo	oper	oper/enda	enda
Types	AN/FC/4V/(PF(1992-2019)/CF(1992-2019)/CV (2006-2016) – only for enfo)	AN/FC/4V	AN/FC/4V	AN/FC
FC base time	0/12 UTC	0/12 UTC	06/18 UTC	18 UTC
Max. time resolution	1-hourly AN/FC mix	3-hourly AN/FC mix (6-hourly AN for public user)	1-hourly AN	1-hourly AN
Highest resolution	~0.1°	0.75° (80km)	0.28125° (31km)	~1.25° (125km)
Levels	137 (starting from 25/06/2013; less levels before, see docu)	60	137	91
Ensemble members	11 (enda); 26 (elda, upto 50 with sythesized doubles); 50 (enfo, since 1996)	-	10 (3-hourly)	10 (3-hourly)
Eta- coordinate vertical velocity	yes	No, only reduced gaussian grid	yes	yes

Schematic overview of access modes



Example application for access from local machine

`Flex_extract` uses so-called "CONTROL" files to define the framework conditions for the data to be extracted and automatically creates the corresponding "MARS requests" which follow ECMWF's own syntax.

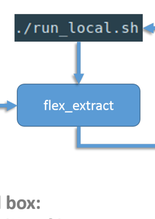
CONTROL_EA5*

```
START_DATE
DTIME 6
TYPE AN AN AN AN
TIME 00 06 12 18
STEP 00 00 00 00
ACCTYPE FC
ACCTIME 06/18
ACCMAXSTEP 12
CLASS EA
STREAM OPER
GRID 0.28125
LEFT 0.
LOWER 0.
UPPER 2.25
RIGHT 2.25
LEVELIST 135/to/137
RESOL 799
ETA 1
PREFIX EA
```

* Minimum number of parameters to be set

run_local.sh (user specification)

```
# ------------------------------------------------------------------
# AVAILABLE COMMANDLINE ARGUMENTS TO SET
#
# THE USER HAS TO SPECIFY THESE PARAMETERS
#
QUEUE='',
START_DATE=20180108
END_DATE=None
DATE_CHUNK=None
JOB_CHUNK=None
BASETIME=None
STEP=None
LEVELIST=None
AREA=None
INPUTDIR='./workspace',
OUTPUTDIR=None
FLEXPARTDIR=None
PP_ID=None
JOB_TEMPLATE='',
CONTROLFILE='CONTROL_EA5',
DEBUG=1
REQUEST=2
PUBLIC=0
# ------------------------------------------------------------------
```



Red box: resulting files as input for FLEXPART; the rest are temporary files

```
ANOG_ML.20180108.16098.16099.grb  FCOG_acc_SL.20180107.16098.16099.grb  flux2018010818  fort.11  fort.21
ANOG_SL.20180108.16098.16099.grb  flux2018010700                       flux2018010900  fort.12  fort.22
ANSH_SL.20180108.16098.16099.grb  flux2018010706                       flux2018010906  fort.13  fort.4
date_time_stepRange.idx           flux2018010712                       flux2018010912  fort.15  mars_requests.csv
EA18010800                        flux2018010718                       flux2018010918  fort.16  OG_OROLSM__SL.20180108.16098.16099.grb
EA18010806                        flux2018010800                       flux2018011000  fort.17  VERTICAL.EC
EA18010812                        flux2018010806                       flux2018011006  fort.18
EA18010818                        flux2018010812                       fort.10         fort.19
```

- *.grb contain the extracted MARS fields
- flux* contain the disaggregated flux fields per time step
- fort.* contain fields grouped by specific characterisations to be read and processed by CONVERT2
- fort.4 namelist file for CONVERT2
- fort.15 resulting file from CONVERT2
- EA* final files of flex_extract. The format corresponds to <prefix>YYMMDDHH, where prefix was defined in CONTROL file

*) Usually all temporary files are deleted (all but <prefix>YYMMDDHH), except flex_extract runs in debug mode.

Parameters to be extracted

FLEXPART expects the following parameters:
- model level parameters: U, V, T, Q, ETADOT, (CIWC+CLWC=QC)
- surface parameters: LNSP/MSL/10u/10v/2T/2D/SD/TCC/SR/Z/SDOR/LSM
- flux data: LSP/CP/SSHF/EWSS/NSSS

Note: Not all meteorological fields and time steps are available for public users. This is taken into account in the sample CONTROL files according to the datasets.

Software environment

Python component:
- Python3 or Anaconda Python3
- numpy
- ecmwf-api-client
- cdsapi
- genshi
- eccodes for standard Python (manually installed or from Linux package) or eccodes from conda

Fortran component:
- Fortran 95 compiler (e.g. gfortran)
- fftw3
- eccodes
- emoslib

Support

- FLEXPART's community website and ticket system: `https://flexpart.eu`
- `flex_extract` Information: `https://www.flexpart.eu/wiki/FpInputMetEcmwf`
- Git-repository: `https://www.flexpart.eu/browser/flex_extract.git`
- Mailing Liste: `flexpart@lists.univie.ac.at`

Outlook

- publish in GMD
- add optional WRF parameter extraction
- finish preparation of online documentation
- add more unit tests
- apply continuous integration with Jenkins
- automatise regression tests
- convert f90 to py
- consider feedback from beta testers (please email me if you want to participate)
- prepare FLEXPART to handle new disaggregated precipitation
- compare FLEXPART deposition fields with old and new disaggregation

`flex_extract` license

References

[1] Anonymous (2019): *The official FLEXPART web site*, `https://www.flexpart.eu/`
[2] Grythe, H.; Kristiansen, N. I.; Groot Zwaaftink, C. D.; Eckhardt, S.; Ström, J.; Tunved, P.; Krejci, R.; and Stohl, A. (2017): *A new aerosol wet removal scheme for the Lagrangian particle model FLEXPART v10*, Geosci. Model Dev., 10, 1447-1466, `https://doi.org/10.5194/gmd-10-1447-2017`
[3] Hittmeir, S.; Philipp, A.; Seibert, P. (2018): *A conservative reconstruction scheme for the interpolation of extensive quantities in the Lagrangian particle dispersion model FLEXPART*, Geosci. Model Dev., 11, 2503-2523, URL: `https://doi.org/10.5194/gmd-2018-333`
[4] Pisso, I.; Sollum, E.; Grythe, H.; Kristiansen, N.; Cassiani, M.; Eckhardt, S.; Arnold, D.; Morton, D.; Thompson, R. L.; Groot Zwaaftink, C. D.; Evangeliou, N.; Sodemann, H.; Haimberger, L.; Henne, S.; Brunner, D.; Burkhart, J. F.; Fouilloux, A.; Brioude, J.; Philipp, A.; Seibert, P.; and Stohl, A. (2019): *The Lagrangian particle dispersion model FLEXPART version 10.3*, Geosci. Model Dev. Discuss., `https://doi.org/10.5194/gmd-2018-333`, in review.
[5] 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.
[6] Stohl, A., C. Forster, A. Frank, P. Seibert, and G. Wotawa (2005): *Technical Note : The Lagrangian particle dispersion model FLEXPART version 6.2*, Atmos. Chem. Phys. 5, 2461-2474.
[7] `https://confluence.ecmwf.int/display/UDOC/User+Documentation`
[8] `https://apps.ecmwf.int/registration/`