Supplement of

Flex_extract v7.1.2 – a software package to retrieve and prepare ECMWF data for use in FLEXPART

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S1. Execution script parameters

S1.1. setup.sh parameters

This shell script defines the command-line parameters for the installation process and executes the Python script install.py for the installation of flex_extract. The following parameters can be set:

| Name: TARGET | Type: String | Value range: local, ecgate, cca, ccb | Default: None |
|--------------|--------------|-----------------------------------|--------------|
| Description: Defines which flex_extract application mode (location of installation) will be used. Local = local mode; ecgate = Remote or Gateway mode, cca/ccb = Remote or Gateway mode. Whether the local mode is for public or member state users doesn’t matter during the installation process. |

| Name: MAKEFILE | Type: String | Value range: any makefile present, according to environment | Default: None |
|---------------|--------------|----------------------------------------------------------|--------------|
| Description: Name of the makefile in Source/Fortran directory to be used for compiling the Fortran program. makefile_ecgate has the configuration for the ecgate environment and makefile_cray has the configuration for the HPC environment. For local server versions there is makefile_local_gfortran which has to be adapted (paths to the ecCodes library) by the user. |
| Name        | Type   | Value range                      | Default          |
|-------------|--------|----------------------------------|------------------|
| **ECUID**   | String | -                                | None             |
| **ECGID**   | String | -                                | None             |
| **DESTINATION** | String | <name>@ generic <scope> | None |
| **GATEWAY** | String | IP address / name               | None             |
| **INSTALLDIR** | String | full path                        | HOME on ECMWF server and current flex_extract root path on local server |
| **JOB_TEMPLAT** | String | installscript.template         | installscript.template |
| **CONTROLFILE** | String | any CONTROL file                 | CONTROL_ERA5     |

**Description**

User id on ECMWF server.

User group id on ECMWF server.

Ectrans destination which is used to transfer files from ECMWF servers to local gateway. This has to be set up by users on the local gateway. See installation instruction for more information.

Name or ip address of member gateway.

Root path where flex_extract should be installed. It will always be set to $HOME on ECMWF servers and on local hosts it will be set to the current flex_extract root path if not set.

The rudimentary template file to create a batch job template for submission to ECMWF servers. Should not be changed since it is optimized for ECMWF server. (Remote and Gateway mode)

The file with all CONTROL parameters.

### S1.2. `run.sh` parameters

This shell script defines the command-line parameters and executes the Python script `submit.py` for running flex_extract. The following parameters can be set:

| Name        | Type   | Value range                      | Default          |
|-------------|--------|----------------------------------|------------------|
| **QUEUE**   | String | ecgate; cca; ccb                | None             |

**Description**

Name of ECMWF server for submission of the job script to its batch system.
| Name         | Type          | Value range                        | Default | Description                                                                 |
|--------------|---------------|------------------------------------|---------|-----------------------------------------------------------------------------|
| **START_DATE** | String [YYYYMMDD] | depends on data set            | None    | The first day of the retrieval period. If **END_DATE** is set, **START_DATE** must be prior to **END_DATE**. |
| **END_DATE**  | String [YYYYMMDD] | depends on data set            | None    | The last day of the retrieval period. This value is optional and if it is not set, it will be automatically set equal to **START_DATE**. For a one day retrieval it has to be equal to **START_DATE**. If set, it has to be greater than or equal to **START_DATE**. |
| **DATE_CHUNK** | Integer       | depends on resolution             | 3       | Maximum number of days retrieved within one MARS request. This number is limited due to maximum allowed memory and time limit for one MARS request. Be careful in changing this number. It can be larger for coarse domains and time intervals but may be too large for very high-resolution retrievals. |
| **JOB_CHUNK**  | Integer       | depends on resolution             | None    | # of days to be retrieved within a single job. Can be selected to start the submission script once and to automatically split the time period into smaller job chunks. For example, it could be very useful if you want to retrieve a month with a resolution of 0.1° and a time resolution of 1 hour. Then only 1 day per job is possible. |
| **BASETIME**  | Integer       | [0;12]                            | None    | This parameter is intended for half-day retrievals. Only half a day will be retrieved starting from **BASETIME** going back 12 hours. E.g. 20180510 with a **BASETIME** = 00 would lead to a data retrieval of 20180509 12h until 20180510 00h. Can be set to 00 or 12 only. |
| **LEVELIST**  | String [start/to/end] | 1/to/[60,91,137] depends on data set | None    | List of vertical levels. It can be a subset of levels but it has to include the maximum level (end) which is the surface. If full list of levels is needed and parameter **LEVEL** is set, the **LEVELIST** parameter is not needed. “end” has to be the maximum number of possible levels and has to be the same as in **LEVEL** (if **LEVEL** specified). |
| **AREA**      | Double [f/f/f/f] | any float within latitude and longitude boundaries | None    | Domain defined as north/west/south/east |
| **INPUTDIR**  | String        | any path                          | None    | Path to the temporary directory for the retrieved GRIB files and other processing files. The temporary directory will be created if it does not already exist. |
### Name: **OUTPUTDIR**
*Type:* String  
*Value range:* any path  
*Default:* None

**Description:**
Path to the final directory where the final FLEXPART ready input files are stored. The final output directory will be created if it does not already exist.

### Name: **PPID**
*Type:* Integer  
*Value range:* -  
*Default:* None

**Description:**
This is the specific parent process id of a single flex_extract run to identify the files. It is the second number in the GRIB filenames. This is usually only necessary if the GRIB data were retrieved and a rerun of the post-processing has to be done. Then PPID is used to select the files.

### Name: **JOB_TEMPLATE**
*Type:* String  
*Value range:* submitscript.template  
*Default:* submitscript.template

**Description:**
Template file which is used remote and gateway modes to create the korn shell job script to be submitted to the batch system on an ECMWF server.

### Name: **CONTROLFILE**
*Type:* String  
*Value range:* any CONTROL file  
*Default:* CONTROL_ERA5

**Description:**
The file with all CONTROL parameters to define a flex_extract retrieval.

### Name: **DEBUG**
*Type:* Integer  
*Value range:* [0,1]  
*Default:* 0

**Description:**
If set to “1” all temporary output files from the MARS requests are kept and some extra information is written out to the log file. Usually all temporary files except the FLEXPART ready input files are deleted at the end of flex_extract.

### Name: **REQUEST**
*Type:* Integer  
*Value range:* [0,1,2]  
*Default:* 2

**Description:**
This parameter allows to write out the MARS requests in a separate file. The requests are stored in the file “mars_requests.csv”. Possible selections are: 1: normal data retrieval; 2: neglect data retrieval and just writes out the MARS requests to the file; 3: retrieve data and write out the MARS requests.

## S2. CONTROL file parameters

### S2.1. User section

### Name: **ECUID**
*Type:* String  
*Value range:* -  
*Default:* None

**Description:**
User id on ECMWF server.

### Name: **ECGID**
*Type:* String  
*Value range:* -  
*Default:* None

**Description:**
User group id on ECMWF server.
### S2.2. Data section

| Name       | Type       | Value range                 | Default | Description                                                                 |
|------------|------------|-----------------------------|---------|-----------------------------------------------------------------------------|
| **DESTINATION** | String    | <name>@ generic <scope>     | None    | Ectrans destination which is used to transfer files from ECMWF servers to local gateway. This has to be set up by users on the local gateway. See installation instruction for more information. |
| **GATEWAY**  | String    | IP address / name           | None    | Name or ip address of member gateway.                                       |
| **CLASS**    | String [xx] | EI, E4, EA, EP, OD         | None    | ECMWF data classification identifier for data sets. EI: ERA-Interim; E4: ERA-40; EA: ERA5; EP: CERA-20C; OD: operational; |
| **DATASET**  | String    | CERA20C, INTERIM           | None    | This keyword has to be defined for retrievals of public data sets ERA-Interim and CERA-20C with ECMWF Web API. Public data are stored in a different MARS database and are available for everyone after registration at ECMWF (see installation plan). Even though ERA5 is also a public data set, the retrieval works differently (with CDS API) and does not need this parameter. |
| **STREAM**   | String [xxxx] | OPER, ENFO, ENDO         | None    | Identifies the forecasting system used to generate the data. Most times the operational data stream OPER is appropriate. Use ENFO for ensemble forecasts and ENDO for CERA data. |
| **EXPVER**   | Integer   | -                           | 1       | Experiment version number. Only necessary for R&D experiments or E-suites; otherwise use 1. |
| **NUMBER**   | String [start/to/end] or Integer | depends on availability | “OFF”  | In most cases this can be set to “OFF”; for access to individual ensemble members of an ensemble forecast the individual numbers have to be selected. Note, however, that model level data are not stored in MARS for individual ensemble members except the control run. They exist only for a few days before they are discarded. For retrieving CERA20C data, a number has to be selected explicitly. Select “0” for the control run. |
### FORMAT

**Name:** FORMAT  
**Type:** String  
**Value range:** [GRIB1, GRIB2]  
**Default:** GRIB1

**Description:**  
Output format (either GRIB1 or GRIB2). Use GRIB2 only when using FLEXPART versions >9.2 or FLEXPART has to be adapted for reading GRIB2. Nowadays, 3D-model level fields are automatically stored on GRIB2 since some GRIB message parameters are not able to be stored in GRIB1 anymore. Surface level fields are always retrieved in GRIB1 and by selecting GRIB2 they are converted to GRIB2 by flex_etract. Be careful with this option, especially if using the ADDPAR parameter to add other fields. Sometimes other surface fields as already defined in flex_etract can’t be converted to GRIB2.

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### S2.3. Data field section

| Name | Type | Value range | Default | Description |
|------|------|-------------|---------|-------------|
| **TYPE** | list of Strings [xx xx . . . xx] | [AN, FC, CV, CF, 4V, PF] | None | A list of field types for each retrieving hour per day. E.g. “AN FC FC AN FC FC” for a day with 3-hourly retrieval (DTIME=3). At 0 and 12 UTC we retrieve analysis fields and at 3, 6, 9, 15, 18 and 21 UTC forecast fields. So far, flex_extract is using ANalysis (AN), ForeCast (FC), Control Forecast (CF), Perturbed Forecast (PF), Calibration/Validation forecast (CV) and 4D Variational analysis (4V). Other types might be also possible but were not tested. The analysis fields are usually (depending on data set) available at 00/06/12/18 UTC. For better temporal resolution, the time in-between the AN fields can be filled with forecasts (FC). Additionally, it is recommended to use analysis fields only at 00 and 12 UTC and fill the rest of the times with other field types, such as forecasts. |
| **TIME** | list of Integer [ii ii . . . ii] | [00 – 23] | None | The time of the corresponding field type (TYPE) in hours. It is important to set the correct forecast times, e.g. in the ERA-Interim data set, forecast times of 00 UTC are normally used to obtain forecast fields between +1 and +11 h; to obtain fields between 13 and 23 UTC, a forecast time of 12 UTC is used. In most cases, there are two forecasts starting per day. TIME has to have the same number of values as TYPE! The start times of forecasts can vary from one data set to another, for example CERA20C has only a single forecast per day (18 UTC). |
| **STEP** | list of Integer [ii ii . . . ii] | [00 – max available STEP in data set] | None | This is the forecast time step in hours for each corresponding field type (TYPE). Counting of the steps starts from the forecast times, e.g. in ERA-Interim, for forecasts verifying at 3, 6, 9 UTC, the STEPS 3, 6 and 9 are used with a forecast TIME 00 UTC. Has to have the same number of values as in TYPE and TIME and has to match with DTIME! For analysis (AN) fields, the STEP has to be 00 always! |
| **MAXSTEP** | Integer | > 24 | None | This parameter allows to retrieve data from forecasts longer than 24 hours. With MAXSTEP >24, the forecasts from different days overlap, the naming scheme of the output files changes from <PREFIX>Yymmdd to <PREFIX>Yymmdd.HH.SSS where HH is the hour of the start of the forecast and SSS is the forecast step in hours. Optional parameter. |
### S2.4. Time section

| Name          | Type        | Value range                  | Default | Description                                                                                                                                                           |
|---------------|-------------|------------------------------|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| **START_DATE**| String [YYYYMMDD] | depends on data set          | None    | The first day of the retrieval period. If **END_DATE** is set, **START_DATE** must be prior to **END_DATE**.                                                            |
| **END_DATE**  | String [YYYYMMDD] | depends on data set          | None    | The last day of the retrieval period. This value is optional and if it is not set, it will be automatically set equal to **START_DATE**. For a one day retrieval it has to be equal to **START_DATE**. If set, it has to be greater than or equal to **START_DATE**.|
| **DTIME**     | Integer     | 1,3,6                        | None    | Time step of retrieved data. Detects TYPE, TIME, STEP, ACCTYPE, ACCTIME according to DTIME. Therefore CONTROL file can have more values than needed. Available resolution in time depends on availability in the data set. Coarser resolution can always be selected. |
| **DATE_CHUNK**| Integer     | depends on resolution        | 3       | Maximum number of days retrieved within one MARS request. This number is limited due to maximum allowed memory and time limit for one MARS request. Be careful in changing this number. It can be larger for coarse domains and time intervals but may be too large for very high resolution retrievals. |
| **BASETIME**  | Integer     | [0;12]                       | None    | This parameter is intended for half-day retrievals. Only half a day will be retrieved starting from BASETIME going back 12 hours. E.g. 20180510 with a BASETIME = 00 would lead to a data retrieval of 20180509 12h until 20180510 00h. Can be set to 00 or 12 only. |

### S2.5. General section

| Name          | Type        | Value range                  | Default | Description                                                                                                                                                           |
|---------------|-------------|------------------------------|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| **DEBUG**     | Integer     | [0,1]                        | 0       | If set to “1” all temporary output files from the MARS requests are kept and some extra information is written out to the log file. Usually all temporary files except the FLEXPART ready output files are deleted at the end of flex_extract. |
| **REQUEST**   | Integer     | [0,1,2]                      | 2       | This parameter allows to write out the MARS requests in a separate file. The requests are stored in the file “mars_requests.csv”. Possible selections are: 1: normal data retrieval; 2: neglect data retrieval and just writes out the MARS requests; 3: retrieve data and write out the MARS requests. |
| Name         | Type                | Value range                     | Default | Description                                                                                                                                                                                                 |
|--------------|---------------------|---------------------------------|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PUBLIC       | Integer             | [0,1]                           | 0       | This specifies the selection of the kind of ECMWF Web Api access and therefore the kind of available data sets. Public data sets (1) and Member-state data sets (0). Selecting the public access method, the DATASET parameter has explicitly to be set to select the data set. (CLASS is not enough.) ATTENTION: For public data sets, users have to accept the licence of the data set to be retrieved. See here for available data sets and their licences: https://software.ecmwf.int/wiki/display/WEBAPI/Available+ECMWF+Public+Datasets |
| OPER         | Integer             | [0,1]                           | 0       | Switch to prepare the operational job script. START_DATE, END_DATE and BASETIME will be prepared with environment variables at ECMWF server. This is only necessary if extraction of half-day retrievals should be done automatically. Specific extra feature which is usually not used by normal flex_extract users. |
| ECSTORAGE    | Integer             | [0,1]                           | 0       | Switch to store FLEXPART ready input files in the ECFS file system. Mind the data limit.                                                                                                                    |
| ECTRANS      | Integer             | [0,1]                           | 0       | Switch to transfer FLEXPART ready input files to the gateway server. The gateway has to be up and running. A destination has to be configured. See installation instructions for more information. |
| PREFIX       | String              | anything                        | EN      | Prefix of FLEXPART ready input files. The files usually have the format <PREFIX>YYMMDDHH.                                                                                                                   |
| ECFSDIR      | String              | any path available              | ectmp:$USER/econdemand/ | The destination directory on ECFS file system if the retrieved data should be stored on ECMWF servers. This is only used if parameter ECSTORAGE is set to “1”.                                                   |
| MAILOPS      | list of String      | any number of mail addresses, separated by comma | [$USER”] | Email list for operational log files on ECMWF servers. The email addresses should be separated by a comma. For the ECMWF server it is enough to give $USER as input. On local system an actual email is preferred to operate correctly. |
| MAILFAIL     | list of String      | any number of mail addresses, separated by comma | [$USER”] | Email list for operational log files on ECMWF servers. The email addresses should be separated by a comma. For the ECMWF server it is enough to give $USER as input. On local system an actual email is preferred to operate correctly. |
### S2.6. Flux data section

| Name       | Type      | Value range                      | Default  |
|------------|-----------|----------------------------------|----------|
| **ACCTYPE**| String [xx] | [FC, CV, CF, 4V, PF]            | None     |

**Description:**
The type of field for accumulated data retrieval. The accumulated data fields are only available from forecast fields. Therefore it is separated from the normal TYPE parameter to allow, for example, retrieval solely of hourly analysis fields in the Era5 data set. For downward compatibility to older versions: if ACCTYPE is not specified, the default value is taken from the second position of the original TYPE parameter (TYPE[2]). NOTE: This is important at the moment the original TYPE parameter is changed from FC to AN for example.

| Name       | Type   | Value range | Default  |
|------------|--------|-------------|----------|
| **ACCTIME** | String | E.g.: Operational, Era-Interim: 00/12 CERA: 18 ERA5: 06/18 | None |

**Description:**
Forecast start times of accumulated fields (fluxes). The starting times of forecast fields varies between different data sets. For downward compatibility to older versions: if ACCTIME is not specified, the default value is 00/12 for ERA-Interim and operational data, 06/18 for ERA5 data and 18 for CERA-20C data.

| Name       | Type   | Value range          | Default  |
|------------|--------|----------------------|----------|
| **ACCMAXSTEP** | Integer | 12, 24 or larger     | None     |

**Description:**
This parameter specifies the maximum step in hours for a specific accumulated forecast start time. For daily retrievals with one forecast time the step shouldn’t be greater than 24h. For two forecast times the ACCMAXSTEP should be 12. If the parameter MAXSTEP is specified to retrieve forecasts longer than 24 hours, this parameter must have the same value. For downward compatibility to older versions: if ACCMAXSTEP is not specified, the default value is set to 12 for ERA5, Era-Interim and operational data or 24 for CERA-20C data, according to one or two forecast times of the data set.

| Name       | Type   | Value range | Default  |
|------------|--------|-------------|----------|
| **RRINT**  | Integer  | [0,1]      | None     |

**Description:**
Switch to select method of disaggregation for precipitation fields. Old method (0) with a simple linear disaggregation or new method (1) with 2 additional subsequent intervals per time interval. For more information see article Hittmeir et al. (2018).

### S2.7. Domain section

| Name       | Type | Value range          | Default  |
|------------|------|----------------------|----------|
| **UPPER**  | String | -90+GRID to 90     | None     |

**Description:**
Latitude of upper right corner of grid area.

| Name       | Type | Value range          | Default  |
|------------|------|----------------------|----------|
| **LOWER**  | String | -90+GRID to 90     | None     |

**Description:**
Latitude of lower left corner of grid area.
| Name   | Type     | Value range                      | Default  |
|--------|----------|----------------------------------|----------|
| **LEFT** | String   | -180+GRID to 180                | None     |
| Description: | | Longitude of lower left corner of grid area. For cyclic (global) grids, use e.g. LEFT = -180 + GRID, RIGHT = 180. For noncyclic grids crossing the dateline (180W), RIGHT may be smaller than LEFT. |
| **RIGHT** | String   | -180+GRID to 180                | None     |
| Description: | | Longitude of upper right corner of grid area. For cyclic (global) grids, use e.g. LEFT = -180 + GRID, RIGHT = 180. For noncyclic grids crossing the dateline (180W), RIGHT may be smaller than LEFT. |
| **LEVEL**   | Integer   | 60, 91, 137 depends on data set  | None     |
| Description: | | Maximum number of vertical levels. ERA-Interim has 60 levels; ERA5 has 137 levels; CERA-20C has 91 levels; Operational data can have different number of model levels depending on the date. Check upfront in the MARS catalogue. If LEVELIST is set, this parameter is not needed. |
| **LEVELIST** | String [start/to/end] | 1/to/[60,91,137] depends on data set | None     |
| Description: | | List of vertical levels. It can be a subset of levels but it has to include the maximum level (end) which is the surface. If full list of levels is needed and parameter LEVEL is set, the LEVELIST parameter is not needed. “end” has to be the maximum number of possible levels and has to be the same as in LEVEL (if LEVEL specified). |
| **GRID**   | Integer [i/i] | 0.1° - appropriate value e.g. 2° | None     |
| Description: | | Horizontal resolution of Latitude/Longitude grid. Best possible resolution varies for different data sets. E.g in operational data it’s 0.1° whereas in Era-Interim it is 0.75°. It can be specified in tenth degrees (1°) or thousandth degrees (1000 for 1°). |
| **RESOL**   | String | depends on GRID                  | None     |
| Description: | | Horizontal resolution of spectral fields. Specifies the desired triangular truncation of retrieved data, before carrying out any other selected post-processing. |
| **SMOOTH** | Integer | approriate number                | 0        |
| Description: | | Spectral truncation of ETADOT after calculation on Gaussian grid. For more information see Sardeshmukh and Hoskins (1984). |
### S2.8. Vertical wind section

| Name     | Type   | Value range | Default | Description |
|----------|--------|-------------|---------|-------------|
| **GAUSS** | Integer | [0,1]       | 0       | A switch to calculate ETADOT from Lat/Lon grid (0) or from Gaussian grid (1). |
| **ACCURACY** | Integer | -           | 24      | Specifies the number of bits per value to be used in the generated GRIB coded fields. |
| **OMEGA** | Integer | [0,1]       | 0       | Retrieve Omega from MARS and put it to file OMEGAyymmddhh. Only useful for debugging reasons. |
| **OMEGADIFF** | Integer | [0,1]       | 0       | Calculate Omega and Dps/Dt from continuity equation for diagnostic purposes and include it in file OMEGAyymmddhh. Only useful for debugging reasons. |
| **ETA**  | Integer | [0,1]       | 0       | Switch to read ETADOT precalculated by ECMWF and multiply it with DPDETA to be compatible with ETADOT calculated from continuity equation. ETADOT calculation from continuity equation on either Gaussian or lat/lon grid is disabled unless ETADIFF is set to 1 as well. ETADOT is available in ERA5, CERA-20C and operational data sets. Precalculated ETADOT is operationally available from September 2008 onwards. However, it is not available in the ERA-40 and ERA-Interim data set. If ETA is selected in the last two data sets, flex_extract fails. |
| **ETADIFF** | Integer | [0,1]       | 0       | Switch to calculate etadot and Dps/Dt from continuity equation for diagnostic purposes and include it in file ETAyymmddhh. Expensive option, only for debugging purposes. |
| **DPDETA** | Integer | [0,1]       | 1       | Switch to multiply etadot with dpdeta – this is the default. In some future version this may change. |
| **ETAPAR** | Integer | 77          | 77      | GRIB parameter number for ETADOT/DPDETA. |
## S2.9. Additional data section

| Name        | Type       | Value range | Default | Description                                                                 |
|-------------|------------|-------------|---------|-----------------------------------------------------------------------------|
| CWC         | Integer    | [0,1]       | 0       | Switch to retrieve cloud water content (sum of cloud liquid water and cloud ice) (1) or not (0). |
| ADDPAR      | String     | [p1/p2/..../pn] | None    | Additional optional surface parameters (2D fields, non-accumulated) Mostly: 27/28/173/186/187/188/235/139/39. Parameters can be specified as the Integer IDs or with the short names. |
| DOUBLEELDA  | Integer    | [0,1]       | 0       | Switch to select the calculation of extra ensemble members for the ELDA stream. It doubles the number of retrieved ensemble members. Each ensemble member is used to create a new synthesized ensemble member by subtracting 2 * ( current time step value - last time step value ) from the current time step value. |

## S3. Quality assurance

This section adds additional information to the main manuscript by adding details about the single tests and the code metrics. The corresponding test data is large and therefore not distributed with the release tarball but rather as an supplement. Download links can be found on the community website.

### S3.1. Unit tests

We used the pytest package which is a part of standard Python as well as the mock package which simulates external dependencies or results for the tests solely. This gives the opportunity to test the good and bad paths in a function and usually a function holds as many unit tests as there are different branches. It is a matter of defining all possible results depending on the input states and verify the expected results. The first set of unit tests were applied for functions from the install and tools modules as well as for the UIOFiles and EcFleXpert class. The details for each test are not described here; their functionality is obvious from the code.

### S3.2. Regression testing for MARS requests

The release comes with a predefined set of CONTROL files explicitly for this test as well as with a set of MARS request reference files from the previous version 7.0.4 and version 7.1. The test can compare any number of MARS request files emerging from a set of CONTROL files. However, one has to make sure that the reference version contains the request files from the same CONTROL files. Results are saved in log files. Instructions on how the test can be conducted are given in a README.md file. The comparison between version 7.0.4 and 7.1 only showed expected differences related to a bug fix in the determination of the time period.
S3.3. Regression testing for GRIB files

The current release version 7.1 includes a minimal set of reference data from version 7.0.4 and 7.1, one for each type of data set. There will be more test data in the future which can then be downloaded from the community website to limit the size of the distributed release tarball. The corresponding reference control files are also distributed with the tarball to enable the retrieval of the data with the new version. This has to be done manually followed by placing the resulting GRIB files in a specific path as described in the README.md file.

S3.4. Functionality and performance tests for the Fortran code

The code package contains a set of reference outputs, and scripts to create the reference output and to run the actual regression tests. It checks for bitwise identity of the output files (data files and standard output written to a log file). A quantitative comparison of the resulting $\hat{\eta}_p$, which would be useful for modifications that affect the results is not yet implemented. The scripts run each test with both the fast and the debug version of the executable. The script for creating the reference also ensures that both yield identical results. In addition, the runtimes are saved to a csv file.

S3.5. Generic test using predefined control files

This has been verified for version 7.1 by manually executing the software with all these files, and inspecting the results produced. Note that public users can only use files ending with .public except for ERA5; they were tested in local public mode. All other cases were tested both in local and in gateway mode. Since the remote mode does not differ much from the gateway mode, only a subset of files were also tested in this mode. Results were evaluated by inspecting the log files for “success” messages and, where possible, with the regression test for GRIB file comparison (Sect. 3.3). Regarding new features, the files were inspected manually for the expected result.

S3.6. Code Metrics

The cyclomatic complexity (CC) is calculated as:

$$CC = E - N + 2P,$$

where $E$ is the number of edges (or also called links) of the graph, $N$ is the number of nodes of the graph and $P$ is the number of connected components (which are sub-graphs from functions independent of the super-graph) (Lacchia, 2019; Beizer, 1990; Sneed et al., 2010). The nodes represent the conditional branch instructions and program junctions, and edges are the segments between such points. This metric was calculated with the radon package (Lacchia, 2019) and provides the CC rank for each function, class and class method. Table 1 shows a summary of all code blocks from version 7.0.4 and 7.1, while Table 2 lists the code blocks which are worse-rated.

The maintainability index (MI), ranking between 0 and 100, is a function of SLOC, CC and the Halstead volume ($V$) (Lacchia, 2019):

$$MI = \max \left[ 0, \frac{100}{171} \left( 171 - 5.2 \ln V - 0.23 \ln CC - 16.2 \ln SLOC + 50 \sin \sqrt{24 C} \right) \right]$$

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Table 1. Number of code blocks (classes, methods, functions) with a specific rank of cyclomatic complexity and the percentage of the total blocks for version 7.1 (116 in total) and 7.0.4 (45 in total). Determined with the Python package radon (Lacchia, 2019).

| Rank | Version 7.0.4 | Version 7.1 |
|------|---------------|-------------|
| A    | 21            | 76          | 65.52 %    |
| B    | 10            | 28          | 24.14 %    |
| C    | 3             | 9           | 7.76 %     |
| D    | 4             | 1           | 0.86 %     |
| E    | 3             | 1           | 0.86 %     |
| F    | 4             | 1           | 0.86 %     |

where C is the fraction of comment lines (converted to radians) (Lacchia, 2019). The Halstead volume is defined as

\[ V = (N_1 + N_2) \log_2 (\eta_1 + \eta_2) \tag{3} \]

with \( \eta_1 \) being the number of distinct operators, \( \eta_2 \) being the number of distinct operands, \( N_1 \) the total number of operators and \( N_2 \) the total number of operands.

The index applies for a complete Python file and Table 3 shows the ranks of version 7.0.4 and 7.1 respectively.
Table 2. Python code blocks and their cyclomatic complexity (CC) which ranks between C and F and their corresponding CC score. The block types are classes (C), class methods (M) and functions (F).

(a) Version 7.0.4

| Block                        | Block type | Rank | CC  |
|------------------------------|------------|------|-----|
| **Class methods**            |            |      |     |
| GribTools.setkeys            | M          | C    | 11  |
| MARSRetrieval.dataRetrieve   | M          | C    | 15  |
| Control                      | C          | D    | 23  |
| EFLexpart.process_output     | M          | D    | 26  |
| EFLexpart                    | C          | E    | 31  |
| EFLexpart.deacc_fluxes       | M          | E    | 34  |
| EFLexpart.retrieve           | M          | F    | 43  |
| EFLexpart._init__            | M          | F    | 49  |
| Control._init__              | M          | F    | 56  |
| EFLexpart.create             | M          | F    | 57  |
|                              | **Module functions** |            |
| install_args_and_control     | F          | C    | 12  |
| getMARSdata                  | F          | D    | 25  |
| install_via_gateway          | F          | D    | 30  |
| interpret_args_and_control   | F          | E    | 34  |

(b) Version 7.1

| Block                        | Block type | Rank | CC  |
|------------------------------|------------|------|-----|
| **Class methods**            |            |      |     |
| EcFlexpart                   | C          | C    | 13  |
| EcFlexpart._create_params    | M          | C    | 13  |
| EcFlexpart._prep_new_rint    | M          | C    | 14  |
| EcFlexpart._create_field_types | M      | C    | 15  |
| MarsRetrieval.data_retrieve  | M          | C    | 16  |
| ControlFile._read_controlfile| M          | C    | 17  |
| EcFlexpart.retrieve          | M          | D    | 25  |
| EcFlexpart.create            | M          | E    | 36  |
| EcFlexpart.deacc_fluxes      | M          | F    | 57  |
|                              | **Module functions** |            |
| install.py::check_install_conditions | F      | C    | 11  |
| install.py::mk_tarball       | F          | C    | 17  |
| disaggregation.py::IA3       | F          | C    | 18  |
Table 3. Maintainability index in increasing order for the Python files of both versions. This was determined with the Python package radon (Lacchia, 2019).

| Version 7.0.4 | File                   | Rank | MI score |
|--------------|------------------------|------|----------|
| Classes/EcFlexpart.py | B | 10.79 |
| Classes/MarsRetrieval.py | A | 26.92 |
| Mods/checks.py | A | 26.15 |
| Classes/MarsRetrieval.py | A | 26.92 |
| Mods/disaggregation.py | A | 28.55 |
| Mods/profiling.py | A | 38.10 |
| Mods/tools.py | A | 38.32 |
| Mods/get_mars_data.py | A | 44.77 |
| install.py | A | 47.33 |
| Mods/prepare_flexpart.py | A | 47.47 |
| Classes/GribUtil.py | A | 57.07 |
| submit.py | A | 58.90 |
| _config.py | A | 77.35 |
| Classes/UioFiles.py | A | 100.00 |

| Version 7.1 | File                   | Rank | MI score |
|--------------|------------------------|------|----------|
| FlexpartTools.py | C | 0.00 |
| opposite.py | A | 45.25 |
| install.py | A | 48.96 |
| getMARSdata.py | A | 56.28 |
| GribTools.py | A | 59.10 |
| submit.py | A | 67.72 |
| prepareFLEXPART.py | A | 71.40 |
| UIOTools.py | A | 85.18 |

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