

# Post-processing and visualizing large climate model data: radionuclide dispersion modelling and High Performance Computing (HPC)

CaSToRC EuroCC Seminar Talk

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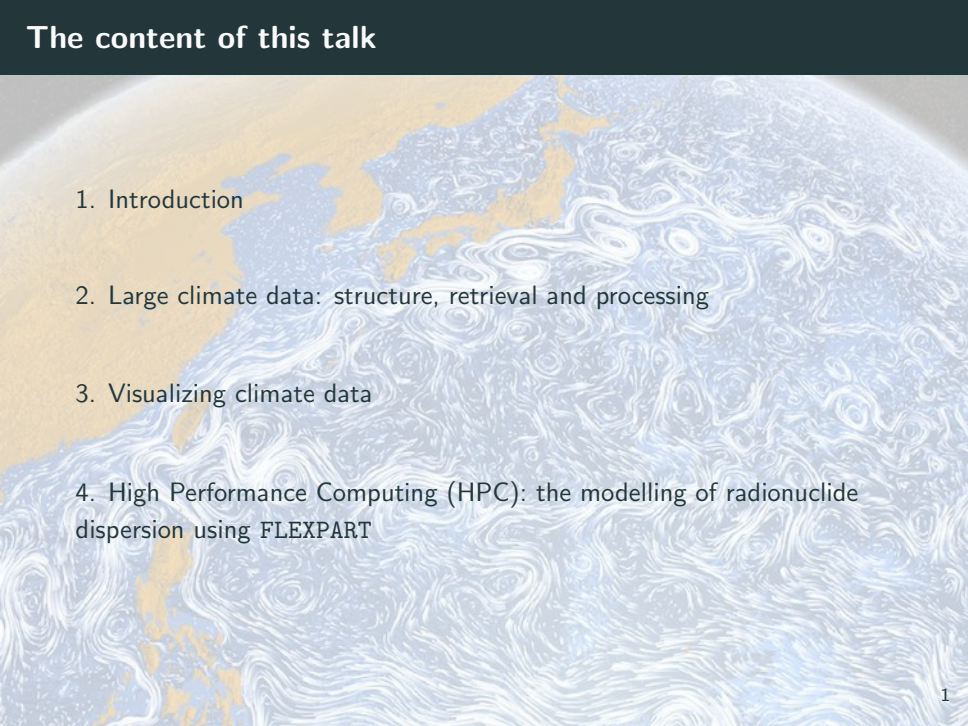
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October 26th, 2021

EPD / CARE-C - The Cyprus Institute

# The content of this talk



1. Introduction
2. Large climate data: structure, retrieval and processing
3. Visualizing climate data
4. High Performance Computing (HPC): the modelling of radionuclide dispersion using FLEXPART

# Introduction

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# Computational Support Specialist – Climate and Atmosphere Research Center (CARE-C)

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## Research Topics

- Atmospheric and climate/earth modelling
- Emission inventories, modelling and analysis
- Dynamical down-scaling of climate change and weather extremes
- Air quality and dust modelling

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## Responsibilities

- Maintenance and management of various geophysical data-sets
- Statistical analysis for the study of temporal and spatial variations of atmospheric and climate data
- Data science and visualisation
- Presentation and interpretation of scientific results

# What turns data into actual **climate** data?

The **short-term** state of the atmosphere is named **weather** (e.g., temperature, precipitation, humidity, cloudiness, wind, et al.), and it can vary from minute to minute and location to location.

**Climate** is a description of the **long-term** pattern of weather conditions at a location. The expression “long-term” usually means 30 years or more, believed to be a good length of time to establish the usual range of conditions at a given location throughout the year.



*The difference between weather variability and long-term climate trends is like the difference between the path of a dog and the path of the person walking the dog*

**Adapted from** : <https://www.climate.gov/maps-data/primer/comparing-climate-and-weather>

**Animation** : <https://youtu.be/e0vj-0im0Lw>

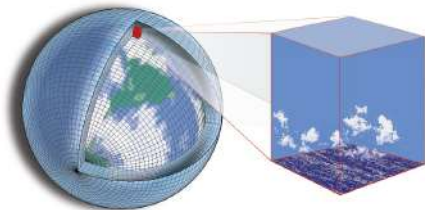
# **Large climate data: structure, retrieval and processing**

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# Climate data: numerical **model** vs. real-world **observations**

## Numerical model

- 361×740 grid points (0.25 deg)  
(e.g.: ds083.3, NCEP, [1])
- 34 vertical levels
- **6-hourly** output, over **15 yrs.**
- multiple quantities (T, p, u, ...)

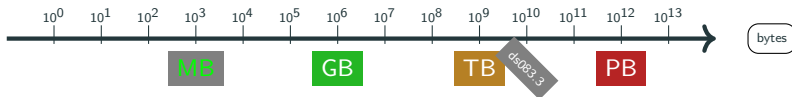


## In-situ observations

- daily to hourly data
- increasing coverage
- smart devices are being progressively used



Extremely large data-sets ( $\approx$  peta-bytes): special binary **formats** needed.



## Selection of common formats

HDF4, HDF5

**Hierarchical Data Format** (NASA)

→ GRIB1, **GRIB2**

**Gridded Binary**

(World Meteorological Organization)

→ **netCDF**

**Network Common Data Form**

(National Center for Atmospheric  
Research)

## Features of binary file:

- non human readable
- sequence of bytes
- memory efficient
- quickly accessible
- cross-platform
- non proprietary format

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**Focus of this talk:** effective post-processing and visualization of large-scale, model-generated climate data. The above format(s) greatly help when post-processing!



## netCDF format is **array-oriented**:

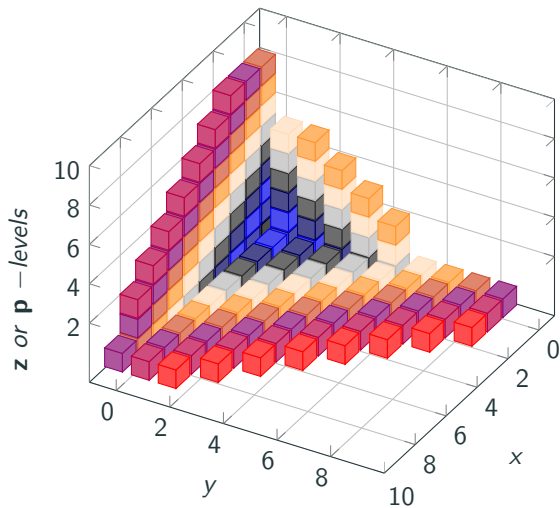
- **Self-Describing**: a netCDF file includes information about the data it contains, i.e.: **attributes** or metadata. (See: [2])
- **Portable**: a netCDF file can be accessed by computers with different ways of storing integers, characters, and floating-point numbers.
- **Scalable**: small subsets of large datasets in various formats may be accessed efficiently through netCDF interfaces, *even from remote servers*.
- **Appendable**: Data may be appended to a properly structured netCDF file without copying the dataset or redefining its structure.



Adapted from: [3] ([www.unidata.ucar.edu/software/netcdf/](http://www.unidata.ucar.edu/software/netcdf/))

More sources: [2], [4], [5].

Example of 3-D array



**data:** numerical values of physical quantities (T, p, v,...)

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**metadata:**

alphanumeric description;  
"data describing data"

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(sub)fields such as:

- size
  - dimensions
  - type
  - unit & time ref
  - space/time convention
- 

collection of self-describing,  
portable objects (See: [4])

## Data describing data – `ncdump`

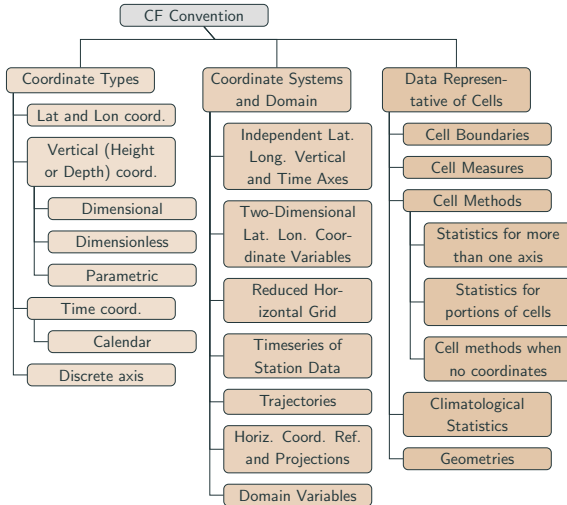
```
# Output file generated with FLEXPART dispersion model
ncdump -h my_netCDF_FileName.nc # "-h" stands for "header only"

dimensions:
    time           = UNLIMITED ; // (336 currently)
    longitude      = 200 ; # nr. of longitudes (gridded)
    latitude       = 280 ; # nr. of latitudes (gridded)
    height         = 2 ; # nr. of vertical levels
    numspec        = 1 ; # number of chem. species (i.e. tracers)
    pointspec      = 1 ; # nr. of release point(s)
    nchar          = 45 ; # string length
    numpoint       = 1 ; # number of receptor(s)

variables:
    int time(time) ;
        time:units = "seconds since 2020-12-01 00:00" ;
        time:calendar = "proleptic_gregorian" ;

    float longitude(longitude) ;
        longitude:long_name = "longitude in degree east" ;
        longitude:axis = "Lon" ;
        longitude:units = "degrees_east" ;
        longitude:standard_name = "grid_longitude" ;
        longitude:description = "grid cell centers" ;
```

# Climate and Forecast (CF) Convention



List of "Software that 'understand' CF" – <https://cfconventions.org/software.html>

Online "CF checker" available – <https://pumatest.nerc.ac.uk/cgi-bin/cf-checker.pl>

More available reference: [6], [7], [8]

## **Findable**

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*Machine-readable metadata are essential for automatic discovery of data-sets and services*

## **Accessible**

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*How can data be accessed, possibly including authentication and authorisation*

## **Interoperable**

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*the data need to interoperate with applications or workflows for analysis, storage, and processing*

## **Reusable**

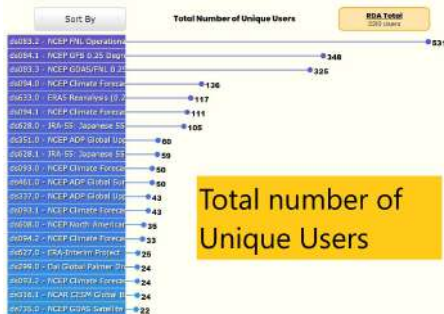
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*Metadata and data should be well-described so that they can be replicated and/or combined in different settings*

# The Research Data Archive (RDA) – free access big data center

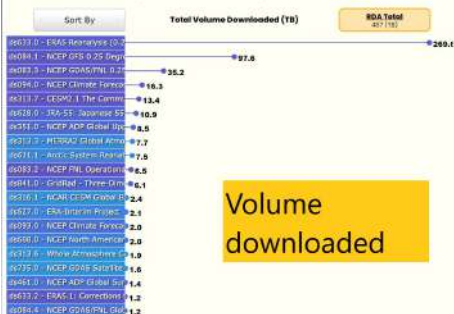
Top 20 most popular datasets by: Month | Year | Citations

## Top 20 datasets in past Month



Top 20 most popular datasets by: Month | Year | Citations

## Top 20 datasets in past Month



```
import rdams_client as rc #import the rdams_client

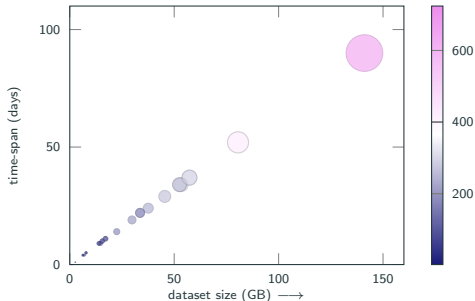
#control file manually, with custom dates, variables, levels and products
idx = rc.submit('controlFile.ct1') #submit a request, and store index
rc.get_status() #check if ready, or more can be submitted
rc.download(idx) #download that index, when ready
```

Eg. datasets: Atmosphere • Ocean • Land cover • Ice sheet cover • Agriculture

NCAR-UCAR: <https://rda.ucar.edu/> – Access requires creation of a user profile (e.g., affiliation and role)

# The Research Data Archive (RDA) – the actual content

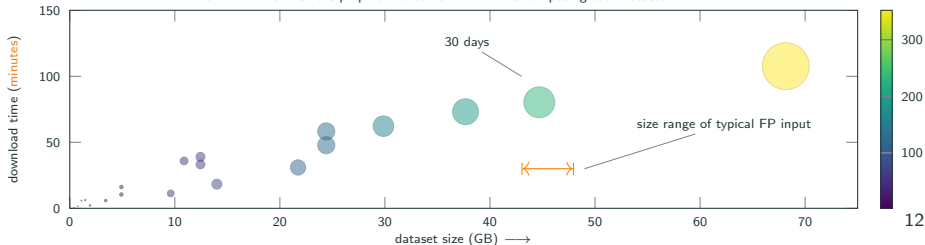
File size vs. its time span - marker color and size is proportional to number of files composing each dataset



Data content, ds083.3 (see [1]):

- **Nr. of variables** : 18
- **Spatial Coverage** : global, @ 0.25 deg
- **Vertical levels** : 34 (isobaric)
- **Products**:
  - Analysis3-hour
  - Accumulation (initial+0 to initial+3)
  - 3-hour Average (initial+0 to initial+3)
  - 3-hour Forecast

ds083.3 - NCEP FNL (Final) operational global analysis and forecast data 0.25-degree grid  
Marker color and size is proportional to number of files composing each dataset



# The fastest ~~pistol~~ climate operator in the west



- **cdo**\* – Climate Data Operator
  - origin: MPI-M, Hamburg, Germany
  - type of data: grib, netCDF
- **eccodes**\*:
  - origin: ECMWF
  - type of data: GRIB 1&2; BUFR 1&2
- **wgrib2**\*:
  - origin: NOAA, Climate Prediction Center
  - type of data: grib2

**Encode and decode.** Open source – \*Python interface

## E.g. of other tools:

- nco: **netCDF operators** – manipulates & analyzes netCDF formats.
- **GeoCAT** Geoscience Community Analysis Toolkit: collection of Python tools related to NCAR Command Language – “swiss knife”

**The spirit of open source & open science!** More references: [9], [10]



## Visualizing climate data

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# NCL - Seasonal mean for radionuclide dispersion

Extracting the near-surface field from initial volume of data:

$$[^{131}I]_{(t_i, x, y, z_0)} = [^{131}I]_{(t_i, x, y, z=0)}$$

Definition of Relative Risk Index (RRI), by normalising the field:

$$RRI_i = \frac{[^{131}I]_{(t_i, x, y, z_0)}}{\max([^{131}I]_{t_i})(x, y, z_0)}$$

Extraction of **monthly mean**:

$$\langle [^{131}I] \rangle_{monthly} = \sum_{i=1}^{nx} \sum_{j=1}^{ny} \sum_{k=1}^{nt} \dots \quad \text{if } j \in [1, 2, 3]$$

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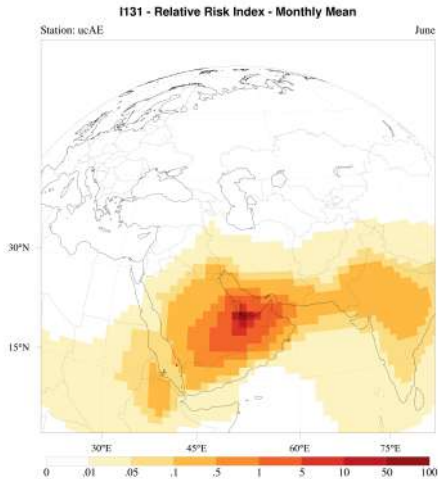
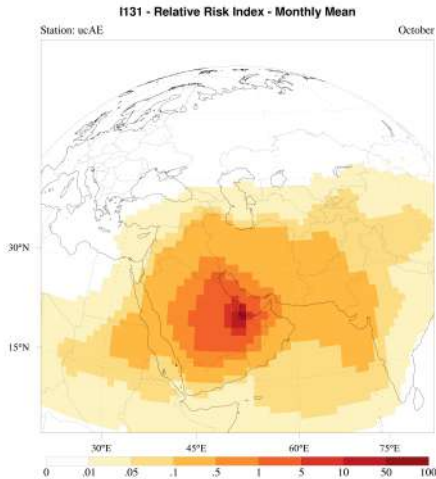
Extraction of **monthly mean**:

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Meanwhile in cdo (either command line or Python,  $\approx 2$  sec/step):

1. `cdo -sellevel,34 -selname,I131 infile outfile`
2. `cdo.expr('norm = I131 / fldmax(I131)'), infile outfile)`
3. `cdo monmean infile outfile`
4. `cdo -O -P 4 -f nc4 -z zip_5 -copy infile outfile`

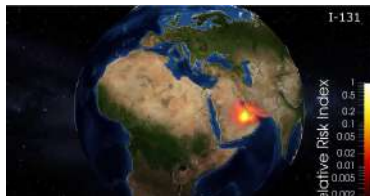
# High-quality (publication ready) maps



Full control over all possible parameters: land boundaries, color-scale, general appearance, output format, etc... – Python compatible!

# Animating results – Paraview

PARAVIEW ([11]) is an open source software for creating high quality animations of scientific data. **Link:** <https://youtu.be/Ks15emMSh7E>

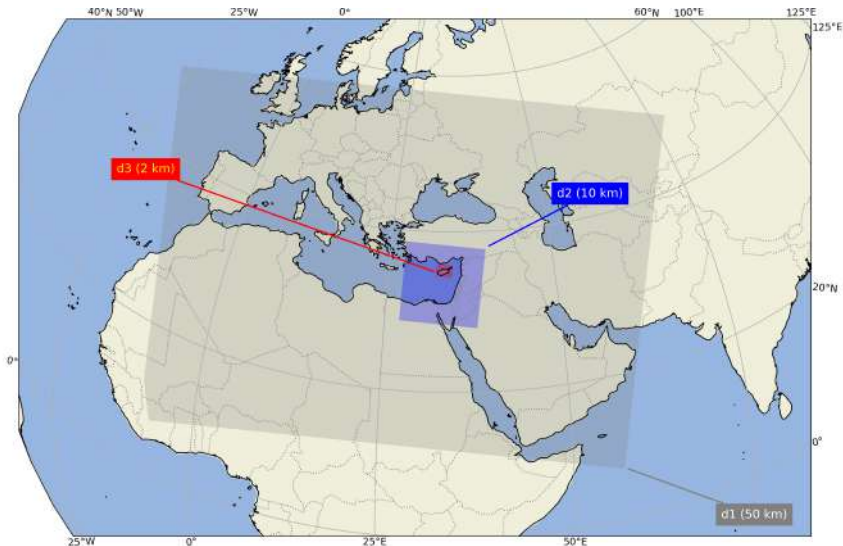


## Iodine – $[^{131}\text{I}]$

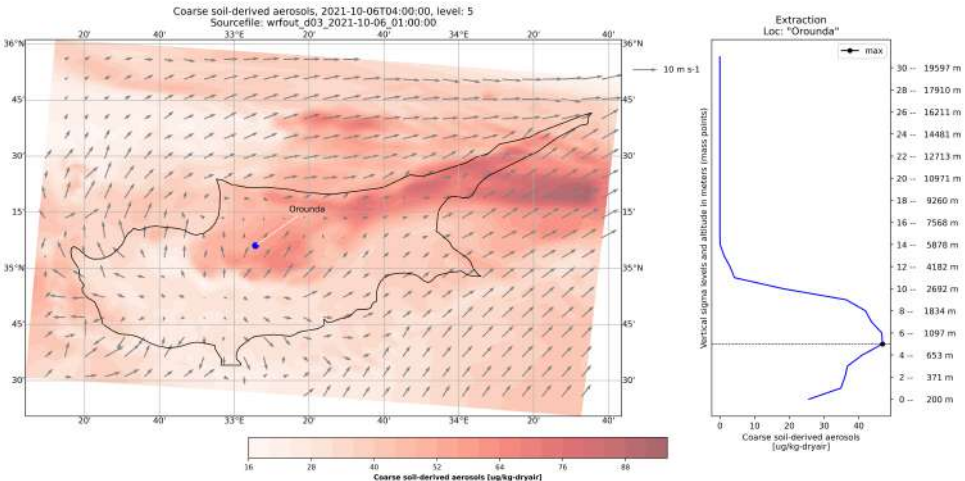
- **gas**
- Half life-time:  $\approx$  **8 days**
- residing in the atmosphere

## Cesium – $[^{137}\text{Cs}]$

- **aerosol**, accumulation (20 yrs)
- Half life-time:  $\approx$  30 yrs decay
- deposited on the ground



# WRF model – dust plumes – maps and vertical profiles



**Aim** – use high-resolution forecast over Cyprus to optimize UAV flight plan with USRL → **Altitude? Trend? Time-window?**

**High Performance Computing  
(HPC): the modelling of  
radionuclide dispersion using  
FLEXPART**

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## ”Release from a hypothetical accident in Akkuyu Nuclear P.P.”

Conclusions: **Topographic factor** was found to play a crucial role:

*”different meteorological data sets are likely to reveal different results even if all other parameters are kept constant” -*

Bilgiç and Gunduz, Journal of Environmental Radioactivity, 2020 ([12]).

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### Improved & more detailed data-set:

High-resolution  
input (ds083.3)

0.5° → 0.25°

6 → 3 hrs

FlexPy package

old, improved

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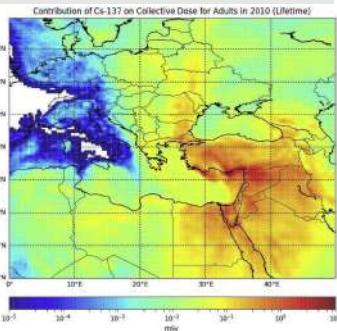
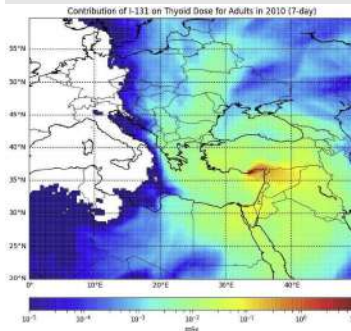
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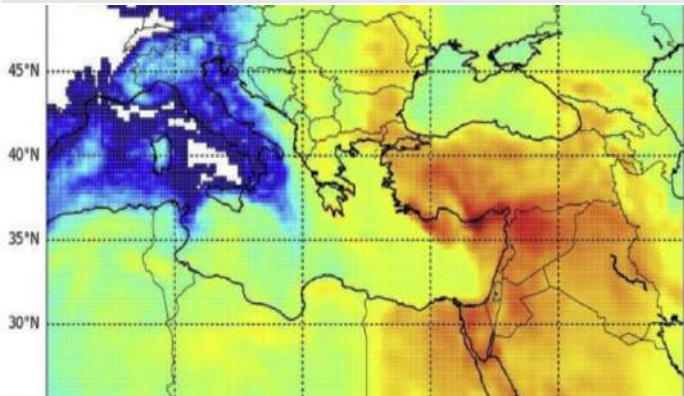
Expansion:

High-resolution  
input (ds083.3)

$0.5^\circ \rightarrow 0.25^\circ$

$6 \rightarrow 3$  hrs

FlexPy package



### **Objective 1**

Create a daily/weekly/seasonal climatology based on multi-year input data. Quickly grab available results/data from the shelf and hand over to policy makers and decision takers...

### **Objective 2**

Reference runs to be compared with available bibliography. Pure research-related speculations...

### **Objective 3**

Reference climatology for future risk assessment – web based services?  
Dissemination etc...

## FLEXPART Lagrangian Dispersion model - v 10.4

- Lagrangian particle dispersion models (LPDM) simulate atmospheric transport & turbulent mixing of gases & aerosols, as well as **dust!**
- Loss processes (radioactive decay, chemical loss, dry/wet deposition) may affect particles and their mass.
- Importance of LPDMs: ability to run backward in time: **trajectories**. Inverse modelling and identification of sources!
- Computational time scales linearly with number of particles used.

Particle trajectory

$\mathbf{X}, \mathbf{v} \rightarrow$  position & wind vector

$t, \Delta t \rightarrow$  time and its increment

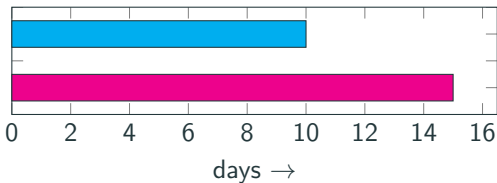
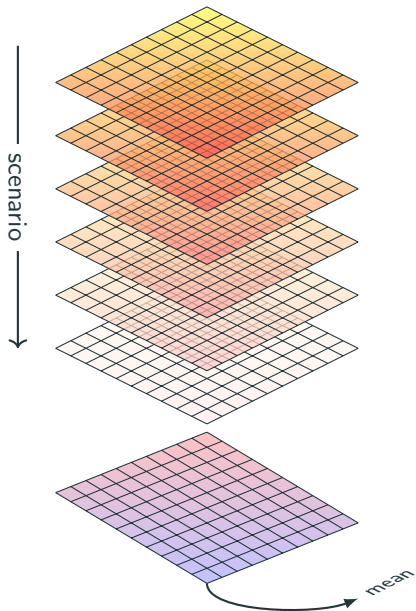
$$\mathbf{X}(t + \Delta t) = \mathbf{X}(t) + \mathbf{v}(x, t) \cdot \Delta t$$

Wet deposition

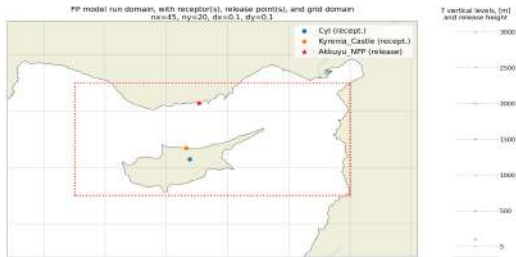
$$m(t + \Delta t) = m(t) \exp(-\Delta t / \beta)$$

References: [13], [14], [15].

# FLEXPART – Climatology based on multi-year input: set-up

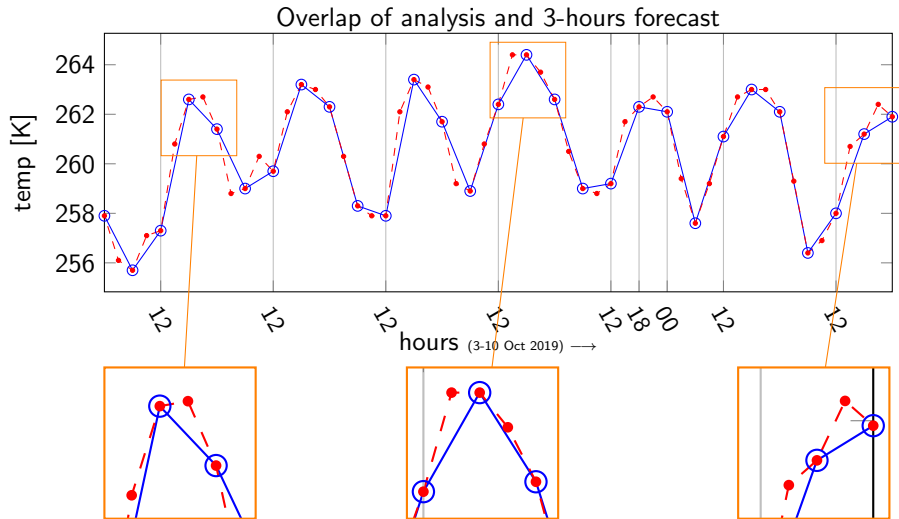


Emission @ Akkuyu (■) and run duration (■)



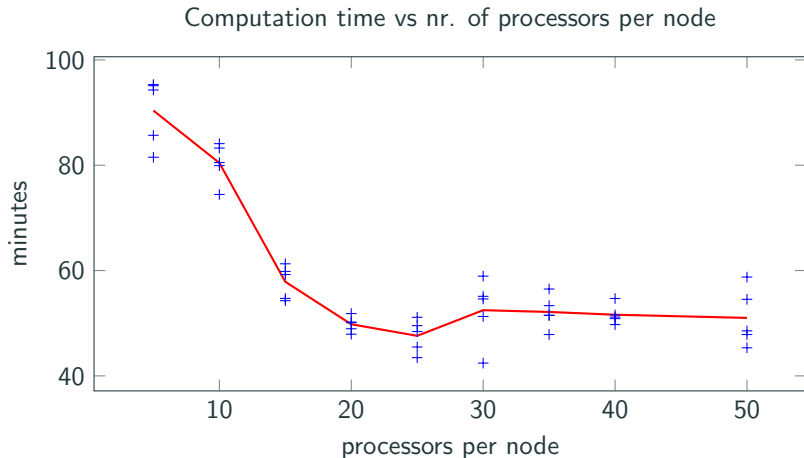
Automatized model set-up – climatology

# Improving temporal resolution with ds083.3: inclusion of f+03



Based on an improved version of Global Forecast System (gfs)

# Performance and CPU resources



Cyl HPC facility – using AMD “Epyc” cluster.



# Inputs – COMMAND file [truncated for brevity]

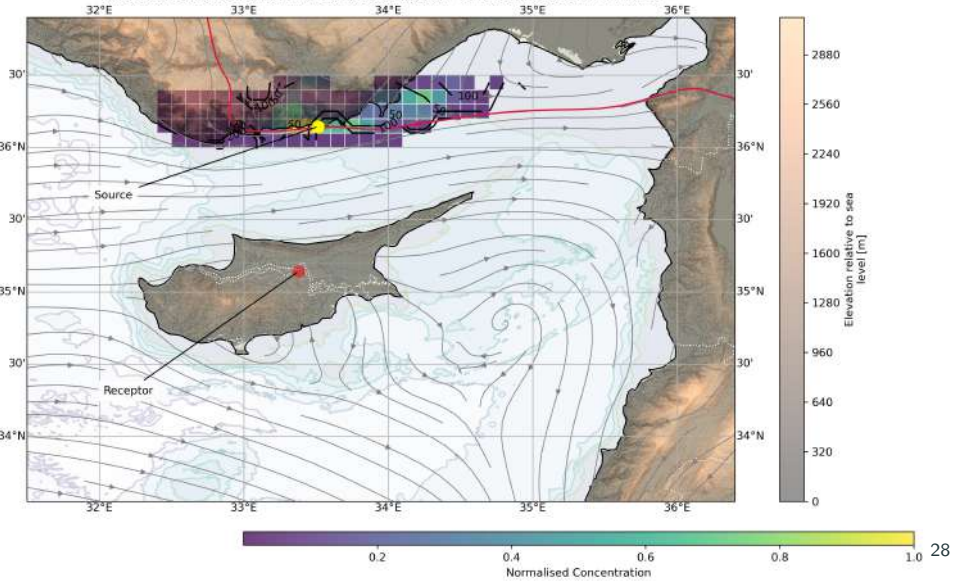
```
*****
* Input file for the Lagrangian particle dispersion model FLEXPART
*           Generated with FlexPy
*****
&COMMAND
LDIRECT=          1, ! Sim. direction  1 (forward), -1 (backward)
IBDATE=          20191001, ! Start date of the simulation  ;
IBTIME=           000000, ! Start time of the simulation  ;
IEDATE=          20191015, ! End date of the simulation  ;
IETIME=          230000, ! End time of the simulation  ;
LOUTSTEP=         3600, ! average concentr. calculated every LOUTSTEP (s)
LOUTAVER=         3600, ! Interval of output averaging (s)
LOUTSAMPLE=       900, ! Interval of output sampling (s),
ITSPLIT=          99999999, ! Interval of particle splitting (s)
LSYNCTIME=        900, ! All processes synchronized to this
IOUT=              9, ! Output type: [1]mass 2]pptv 3]1&2 4]plume 5]1&
IPOUT=             1, ! Particle position output: 0]no 1]every output
LSUBGRID=          0, ! Increase of ABL heights due to sub-grid scale
LCONVECTION=       1, ! Switch for convection parameterization;
LAGESPECTRA=       0, ! Switch for calculation of age spectra
IFLUX=             0, ! Output of mass fluxes through output grid box
MDOMAINFILL=       0, ! Switch for domain-filling, if limited-area par
IND_SOURCE=        1, ! Unit for source : [1]mass 2]mass mixing ratio
IND_RECEPTOR=    1, ! Unit for receptor: [1]mass 2]mass mixing ratio
MQUASILAG=         0, ! Quasi-Lagrangian mode to track individual numbe
```

# OUTPUTs – OUTGRID file [truncated for brevity]

31.50000	GEOGRAFICAL LONG. OF LOWER LEFT CORNER OF OUTPUT GRID
OUTLONLEFT	(left boundary of first grid cell - non its centre)
34.50000	GEOGRAFICAL LAT. OF LOWER LEFT CORNER OF OUTPUT GRID
OUTLATLOWER	(lower boundary of first grid cell - non its centre)
45	NUMBER OF GRID Pts IN X DIRECTION (=No. of cells+1)
NUMXGRID	
20	NUMBER OF GRID Pts IN Y DIRECTION (=No. of cells+1)
NUMYGRID	
0.10000	GRID DISTANCE IN X DIRECTION
DXOUTLON	
0.10000	GRID DISTANCE IN Y DIRECTION
DYOUTLAT	
5	NUMBER OF LEVELS
LEVEL 1	HEIGHT OF LEV (UPPER BOUNDARY)
500	
LEVEL 2	HEIGHT OF LEV (UPPER BOUNDARY)
1000	
LEVEL 3	HEIGHT OF LEV (UPPER BOUNDARY)
1500	
LEVEL 4	HEIGHT OF LEV (UPPER BOUNDARY)

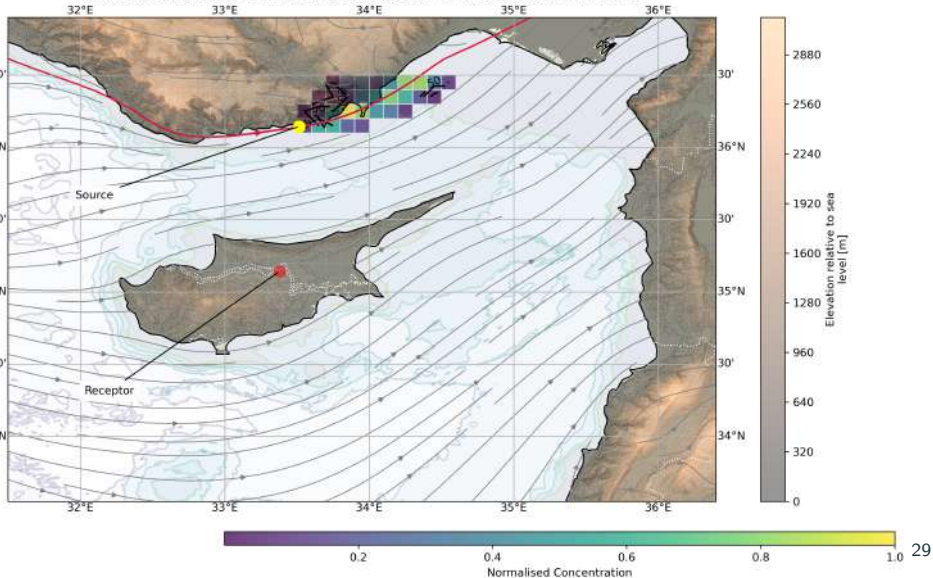
# FLEXPART results – Iodine – normalised concentration 1day

Time: 2019-10-02T00:00:00.000000000, z = 50.0 -- Altitude of max normalised concentration  
Simulation start: 2019-10-01T01:00:00.000000000 -- simulation duration: 23 hours



# FLEXPART results – Iodine – normalised concentration 2 days

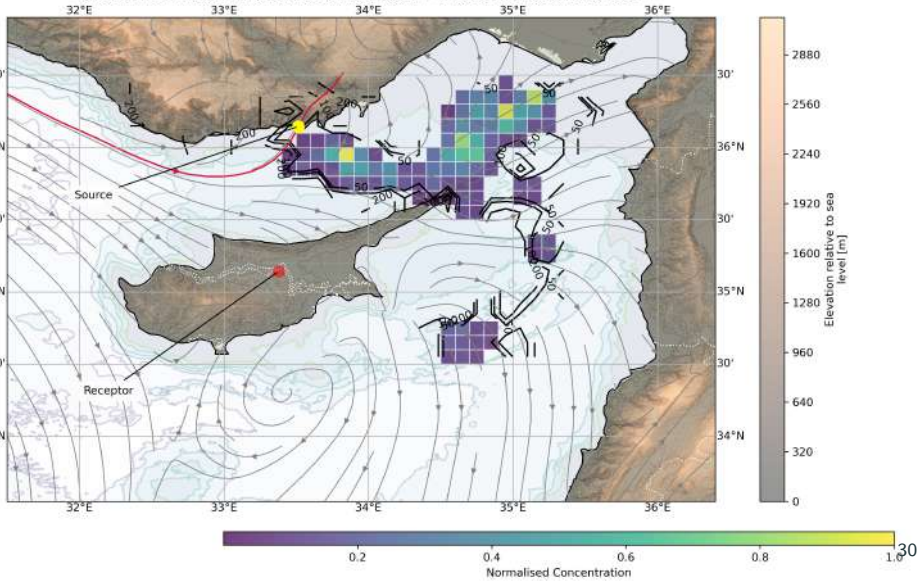
Time: 2019-10-03T00:00:00.000000000, z = 50.0 -- Altitude of max normalised concentration  
Simulation start: 2019-10-01T01:00:00.000000000 -- simulation duration: 47 hours



# FLEXPART results – Iodine – normalised concentration 1/3

Time: 2019-10-09T09:00:00.000000000, z = 0.5 -- Altitude of max normalised concentration

Simulation start: 2019-10-01T01:00:00.000000000 -- simulation duration: 200 hours

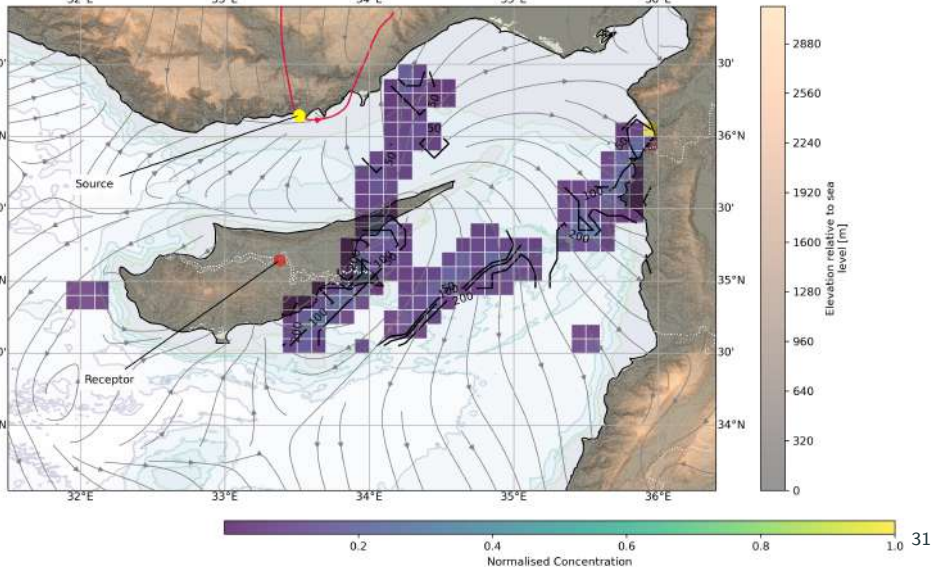


# FLEXPART results – Iodine – normalised concentration <sup>2/3</sup>

Time: 2019-10-12T12:00:00.000000000, z = 100.0 -- Altitude of max normalised concentration

Simulation start: 2019-10-01T01:00:00.000000000 -- simulation duration: 275 hours

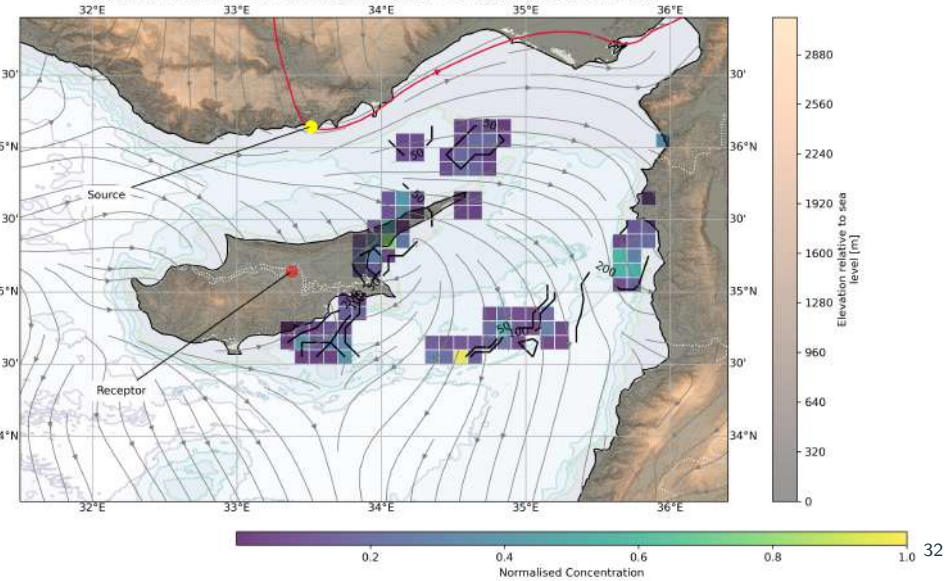
32°E 33°E 34°E 35°E 36°E



# FLEXPART results – Iodine – normalised concentration 3/3

Time: 2019-10-12T15:00:00.000000000, z = 100.0 -- Altitude of max normalised concentration

Simulation start: 2019-10-01T01:00:00.000000000 -- simulation duration: 278 hours



*Questions are welcome*

*Backup slides on following pages*



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Web: [cyi.ac.cy](http://cyi.ac.cy) — [emme-care.cyi.ac.cy](http://emme-care.cyi.ac.cy)



- [1] National Centers for Environmental Prediction, National Weather Service, NOAA, U.S. Department of Commerce, “NCEP GDAS/FNL 0.25 Degree Global Tropospheric Analyses and Forecast Grids,” Boulder CO, 2015. [Online]. Available: <https://doi.org/10.5065/D65Q4T4Z>
- [2] NOAA, “World Ocean Database ragged array netCDF format.” [Online]. Available: [https://www.nodc.noaa.gov/OC5/WOD/netcdf\\_descr.html](https://www.nodc.noaa.gov/OC5/WOD/netcdf_descr.html)
- [3] UniData.ucar.edu, “Network common data form (netcdf).” [Online]. Available: <https://www.unidata.ucar.edu/software/netcdf/>
- [4] netCDF, “An introduction to netcdf.” [Online]. Available: <https://www.unidata.ucar.edu/software/netcdf/docs/>

## References ii

- [5] NOAA, "What is netcdf?" [Online]. Available: <https://www.esrl.noaa.gov/psd/data/gridded/whatsnetCDF.html>
- [6] CF Community, "CF conventions and metadata." [Online]. Available: <http://cfconventions.org/>
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# Backup slides



## cdo – some more insight with examples

```
cdo -ntime <infile>          – Display number of timesteps of a file  
cdo -selname,tas <in> <out>   – Select variable tas from file  
cdo -seltimestep,1/12 <in> <out> – Select a time range (1 → 12)  
cdo -invertlat <in> <out>     – Invert latitudes from N-S to S-N
```

Interpolate model levels to pressure levels:

```
cdo -m12pl,92500,85000,50000,20000 <in> <out>
```

Create a file with masked ocean:

```
cdo -setrtomiss,-20000,0 -topo topo-Land.grb ←
```

Interpolate 6-hourly data to 1-hourly data:

```
cdo -inttime,6 <infile> <outfile>
```

→ operators can be combined and concatenated!

```
cdo -timmean -yearsum -setrtoc,0,15,0 -selname,depth ...  
    -selmon,1,2,3 -selyear,1960/1969 <infile> <outfile>
```

## wgrib2 - slice and dice grib2 format (encode and decode!)

**Question:** I have a grib2 file that contains information at global scale. Using wgrib2, I want to extract a subset from it based on user-provided latitude(s) and longitude(s). **How can I do that?**

```
wgrib2 INput.grb 30:35:.2 31:34:.2 OUTput.grb2 grib
```

INput.grb	- original input file name
30:35:.2	- $lat_i, lat_e, \Delta_{lat}$
31:34:.2	- $lon_i, lon_e, \Delta_{lon}$
OUTput.grb	- output file name
grib	- format to be encoded in

Confront with:

```
cdo -sellonlatbox,lon_i,lon_e,lat_i,lat_e INput.grb OUTput.grb
```

## ecCodes – effective use to compare two suspicious .grb files

**Question:** From **Research Data Archive**, download *exact* same input climate data, via (a) GUI and (b) control file. Model would accept only one of them. – **Why?**

"OUTPUT grid outside mother domain" – FLEXPART

```
long [totalLength]: [945255] != [1297979]
long [latitudeOfFirstGridPoint]: [90000000] != [-90000000]
long [longitudeOfFirstGridPoint]: [0] != [180000000]
long [latitudeOfLastGridPoint]: [-90000000] != [90000000]
long [longitudeOfLastGridPoint]: [359750000] != [179750000]
long [scanningMode]: [0] != [64] ([00000000] != [01000000])
long [parameterCategory]: [2] != [0]
long [parameterNumber]: [2] != [0]
string [typeOfFirstFixedSurface]: [sfc] != [pl]
long [scaledValueOfFirstFixedSurface]: [10] != [200]
long [dataRepresentationTemplateNumber]: [3] != [0]
[missingValueManagementUsed] not found in 2nd field
```

Beside coordinate grid, more metadata being inspected (here, only a few shown...) 41



# Parameter identification – grib v.1 vs grib v.2 definition tables

## GRIB2 - GRIB1 Local Parameter Conversion Table

Revised 02/27/2009

Red text depicts changes made since 03/25/2008

The following table contains a list of GRIB1 locally defined NCEP parameters and their GRIB2 equivalent.

GRIB2			Parameter Name	GRIB1	
Product Discipline	Category	Parameter Number		Parameter Table #	Parameter Number
Sect 0 Octet 7	Sect 4 Octet 10	Sect 4 Octet 11		Sect 1 Octet 4	Sect 1 Octet 5
0	0	0	Temperature	3 (SST)	11
0	0	15	Virtual potential temperature	2	189
0	0	192	Snow Phase Change Heat Flux	2	220
0	0	193	Temperature tendency by all radiation	2	216
0	1	22	Cloud Water Mixing Ratio	2	153
0	1	23	Ice mixing ratio	2	178
0	1	24	Rain Water Mixing Ratio	2	170
0	1	25	Snow Water Mixing Ratio	2	171
0	1	32	Graupel mixing ratio	2	179
0	1	192	Categorical Rain	2	140
0	1	193	Categorical Freezing Rain	2	141
0	1	194	Categorical Ice Pellets	2	142
0	1	195	Categorical Snow	2	143
0	1	196	Convective Precipitation Rate	2	214
0	1	197	Horizontal Moisture Divergence	2	135
0	1	199	Potential Evaporation	2	228
0	1	200	Potential Evaporation Rate	2	145
0	1	201	Snow Cover	2	238
0	1	202	Rain Fraction of Total Liquid Water	129	131
0	1	203	Rime Factor	129	133
0	1	204	Total Column Integrated Rain	129	138
0	1	205	Total Column Integrated Snow	129	139
0	1	206	Total Icing Potential Diagnostic	2	186
0	1	207	Number concentration for ice particles	2	198

GRIB1: Element coding by element and table

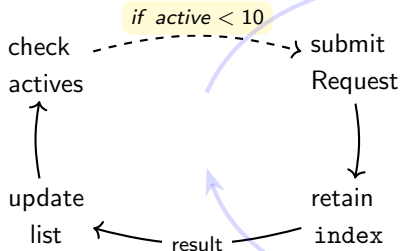
- Eg: temperature is element=11 in table=3 (WMO)

GRIB2: Element coding by a triplet: discipline, category, parameter

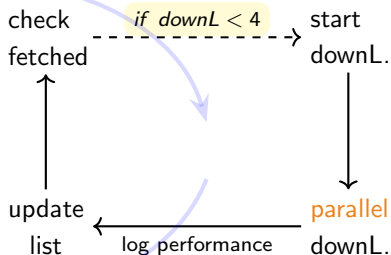
- Eg: temperature is (0,0,0)

# The Python API client – 2 steps workflow

## 1- Submitting requests to RDA



## 2- Bringing completed request home



**Submission constrain:** max number of active requests per user being processed (RDA side) **equals 10**.

**Download constrain:** max number of active datasets being downloaded in parallel, **should not exceed equal 3**.

```
from rda_client import submit, checkStatus, download, authenticate
```