Atmospheric Retrievals in a Modern Python Framework

Mario Echeverri Bautista[1], Anton Verhoef[1], Ad Stoffelen[1], Maximilian Maahn[2]

(1) KNMI
(2) Leipzig University, Institute for Meteorology

mario.echeverribautista@knmi.nl

https://github.com/deweatherman

Koninklijk Nederlands Meteorologisch Instituut
Ministerie van Infrastructuur en Milieu

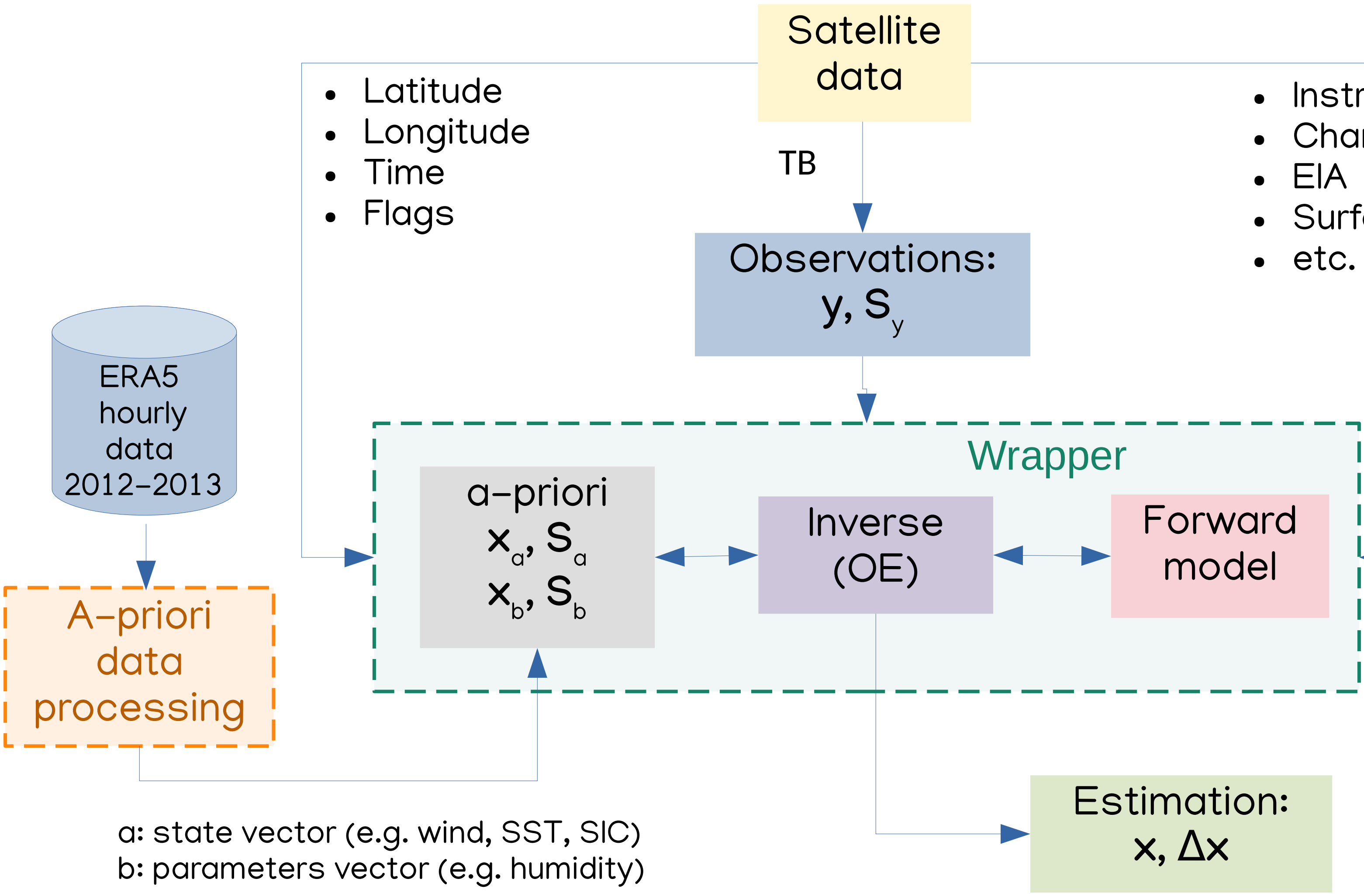
UNIVERSITÄT LEIPZIG

EGU General Assembly 2022, Vienna, Austria, 23–27 May 2022, EGU22-13556

Today's story:

- The main idea
- From Observations to Atmosphere
- Going at scale using Pangeo
- Ongoing activities
- Wrap up

The OE pipeline:



a: state vector (e.g. wind, SST, SIC)
b: parameters vector (e.g. humidity)

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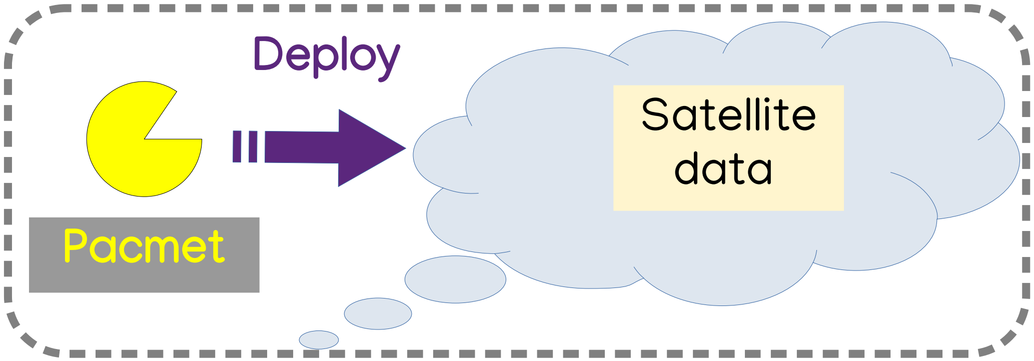
Data-centered framework:



- We want to process a bunch of data on a "cloud".
- Data downstream is increasing with time, solution needs to scale up easily.
- Software is modular; components are "easily" deployed.
- Desirable: Interface with modern Machine Learning libraries possible.

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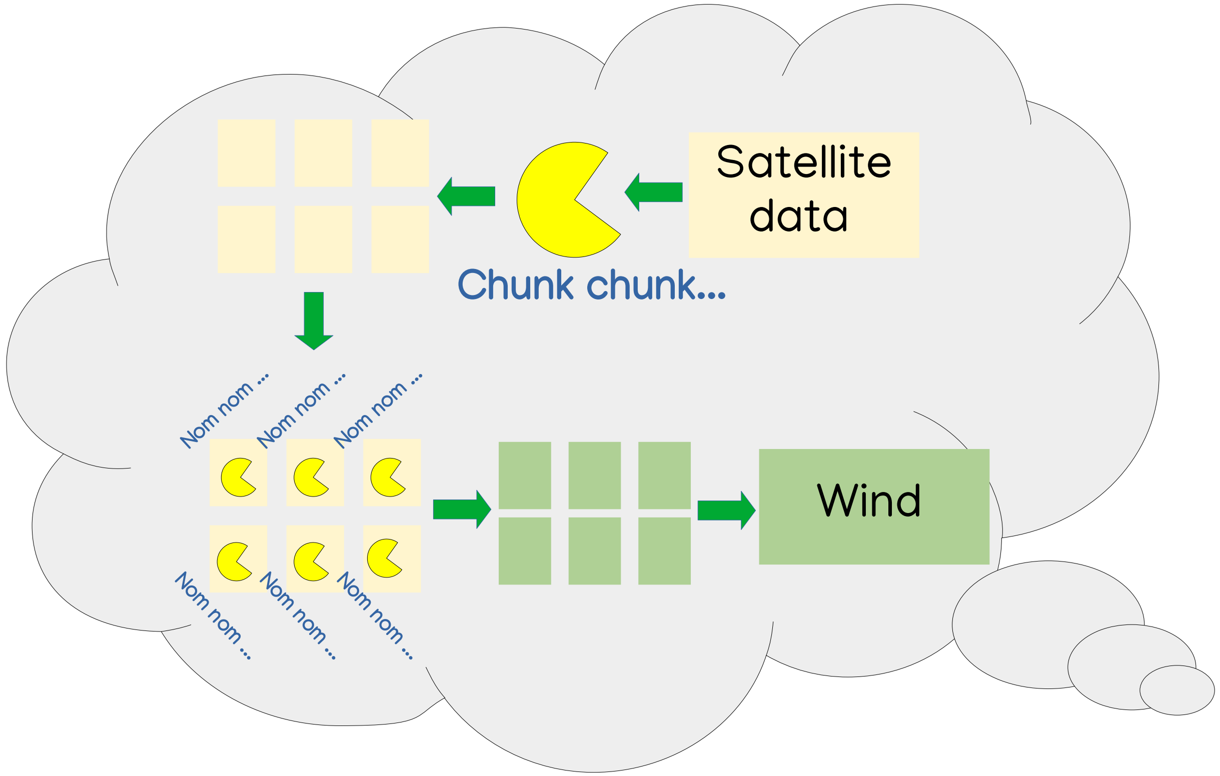
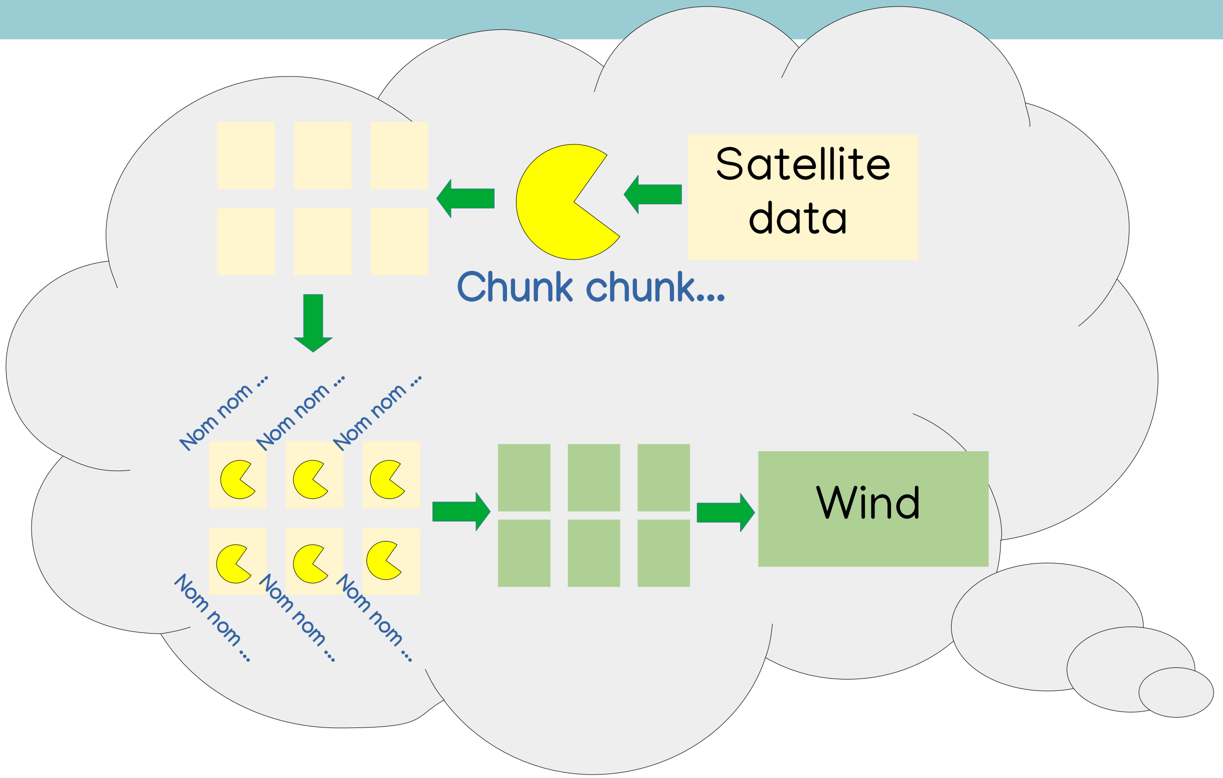
Data-centered framework: wind example



Data-centered framework: caveats



- **Chunking** is a logical operation, i.e. inexpensive*.
- **"Nom nom…"** refers to the processing our *chunks* of data.
- Number of *chunks* do not need to be same as number of workers:

* It generate tasks to be performed, this is not a 'live' operation, but the tasks are to be performed at some point. The message, do not overdo with chunking.

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Data Model and Data Formats

- We use xarray[1] as data interface.
- xarray follows the NetCDF data model (thus it follows CF conventions[2]):
  - **Self-Describing.** A netCDF file includes information about the data it contains.
  - **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.
  - **Sharable.** One writer and multiple readers may simultaneously access the same netCDF file.
  - **Archivable.** Access to all earlier forms of netCDF data will be supported by current and future versions of the software.
- This is highly beneficial in terms of embracing FAIR principles.
- xarray's API handles among others NetCDF, GRIB and zarr.
- xarray can be seen as a multidimensional Pandas and labeled Numpy.

1) https://docs.xarray.dev/en/stable/index.html
2) https://cfconventions.org/cf-conventions/cf-conventions.pdf

Data Model and Data Formats: examples

GRIB (ERA5)

xarray.Dataset

- Dimensions: (**time**: 96, **step**: 2, **isobaricInhPa**: 37, **latitude**: 724, **longitude**: 1440)

▾ Coordinates:

number	()	int64	0
time	(time)	datetime64[ns]	2014-01-01T0...
step	(step)	timedelta64[ns]	06:00:00 18:0...
isobaricInhPa	(isobaricInhPa)	float64	1e+03 975.0 9...
latitude	(latitude)	float64	90.0 89.75 89....
longitude	(longitude)	float64	-180.0 -179.8 ....
valid_time	(time, step)	datetime64[ns]	dask.array<ch...
surface	()	float64	0.0

▾ Data variables:

t	(time, step, isobaricInhPa, latitude, longitude)	float32	dask.array<ch...
q	(time, step, isobaricInhPa, latitude, longitude)	float32	dask.array<ch...
u10n	(time, step, latitude, longitude)	float32	dask.array<ch...
v10n	(time, step, latitude, longitude)	float32	dask.array<ch...
sp	(time, step, latitude, longitude)	float32	dask.array<ch...
t2m	(time, step, latitude, longitude)	float32	dask.array<ch...
lsm	(time, step, latitude, longitude)	float32	dask.array<ch...
skt	(time, step, latitude, longitude)	float32	dask.array<ch...

▾ Attributes:

GRIB_edition :	1
GRIB_centre :	ecmf
GRIB_centreDe...	European Centre for Medium-Range Weather Forecasts
GRIB_subCentre :	0
Conventions :	CF-1.7
institution :	European Centre for Medium-Range Weather Forecasts
history :	2022-03-11T10:35 GRIB to CDM+CF via cfgrib-0.9.9.0/ecCodes-2.22.1 with {"source": "/home/mario/Data/Covariance_means/MARS_api_data/ERA5_data/datasets/profiles_2014UC.grib", "filter_by_keys": {}, "encode_cf": ["parameter", "time", "geography", "vertical"]}

NetCDF (*CMSAF-ish)

xarray.Dataset

- Dimensions: (**time**: 45505, **scene_across_track**: 90, **scene_channel**: 5)

▾ Coordinates:

scene_across_...	(scene_across_track)	int32	1 5 9 13 17 ... 34...
scene_channel	(scene_channel)	int64	11 12 13 14 15
time	(time)	datetime64[ns]	2014-09-09 ... 2...

▾ Data variables:

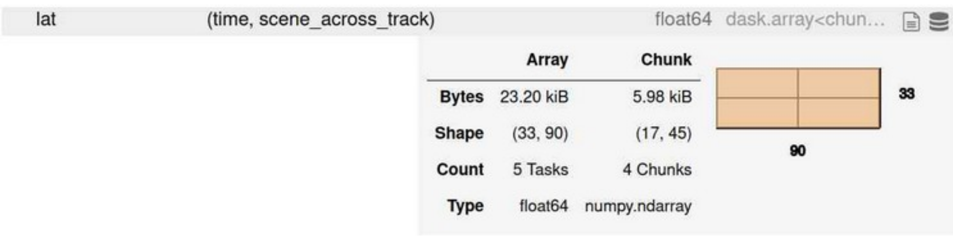
lat	(time, scene_across_track)	float64	dask.array<chun...
lon	(time, scene_across_track)	float64	dask.array<chun...
eia	(time, scene_across_track)	float32	dask.array<chun...
sft	(time, scene_across_track)	float32	dask.array<chun...
tb	(time, scene_across_track, scene_channel)	float32	dask.array<chun...
global_channel...	(scene_channel)	int32	dask.array<chun...
channel_uncert...	(scene_channel)	float32	dask.array<chun...
wind	(time, scene_across_track)	float32	dask.array<chun...
wind_err	(time, scene_across_track)	float32	dask.array<chun...
chiSquareTest1	(time, scene_across_track)	float32	dask.array<chun...
chiSquareTest2	(time, scene_across_track)	float32	dask.array<chun...
chiSquareTest3	(time, scene_across_track)	float32	dask.array<chun...
chiSquareTest4	(time, scene_across_track)	float32	dask.array<chun...

▾ Attributes:

title :	Environmental Scene 1
comment :	feedhorn channels: h19, v19, v22
elevation_offset...	0.4
azimuth_offset_...	-0.3

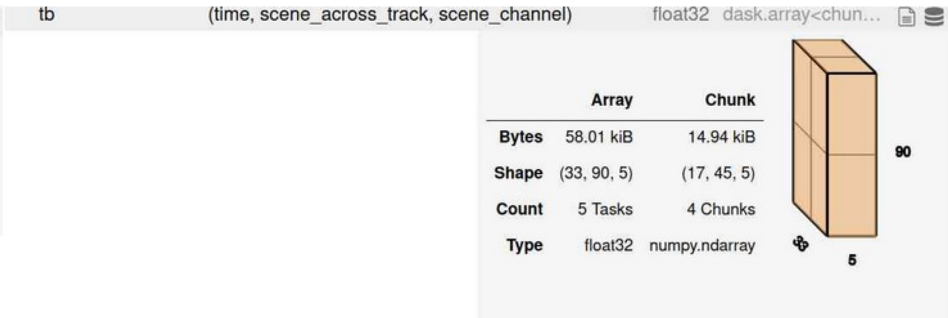
*TB from CMSAF: https://wui.cmsaf.eu/safira/action/viewDoiDetails?acronym=FCDR_MWI_V003

Big data, chunks and processing: Nom nom...



lat (time, scene_across_track) float64 dask.array<chun...

	Array	Chunk
Bytes	23.20 kiB	5.98 kiB
Shape	(33, 90)	(17, 45)
Count	5 Tasks	4 Chunks
Type	float64	numpy.ndarray

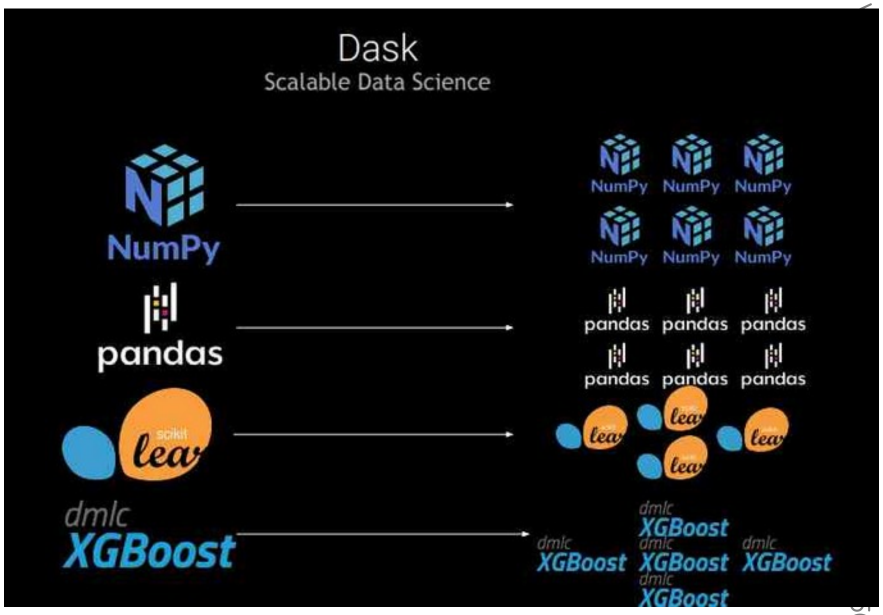


tb (time, scene_across_track, scene_channel) float32 dask.array<chun...

	Array	Chunk
Bytes	58.01 kiB	14.94 kiB
Shape	(33, 90, 5)	(17, 45, 5)
Count	5 Tasks	4 Chunks
Type	float32	numpy.ndarray

- ➢ xarray uses Dask[1] under the hood in order to handle big datasets
- ➢ Divide and conquer strategy: divide dataset in chunks and process

From 2



1) https://docs.dask.org/en/stable/
2) https://www.nvidia.com/en-us/glossary/data-science/dask/

Our application: wind retrieval

- Wind retrievals using optimal estimation and radiometer observations:
  - We use pyOptimalEstimation for performing the retrieval (core computation); open source project (ME contributor).
  - We use pyResample (pyTroll) for re-sampling (when needed).
  - We use xarray + Dask for multi-dimensional labeled datasets handling[1] and high level parallelization[2] .
  - We use RTTOV from NWPSAF as radiative transfer model (i.e. forward model).

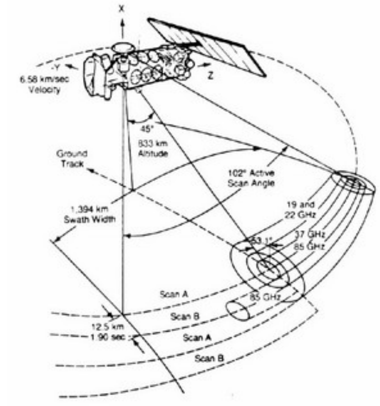
1) Handling includes Numpy and Pandas native support + Dask chunking

2) High level parallelization includes creation of cluster of workers and scheduling tasks to be executed.

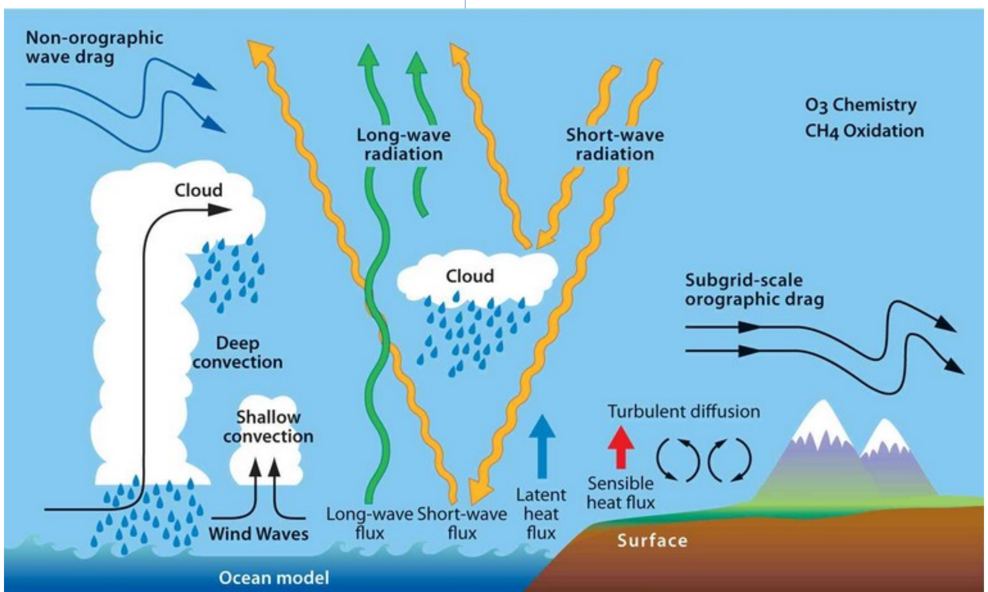
Wind retrievals: Radiative transfer (forward model)

Top of the Atmosphere: TOA

Observations: Brightness temperature (TB)



profiles: Temp., Hum., Press., etc.



...

A **forward** model connects the unknowns with the observations:

TB = F(f, θ, b, *profiles*, *NSWS*)

Surface of the ocean

Surface unknowns: Wind speed at 10m height

*From: https://www.ecmwf.int/en/research/modelling-and-prediction/atmospheric-physics

Optimal Estimation (OE): inversion

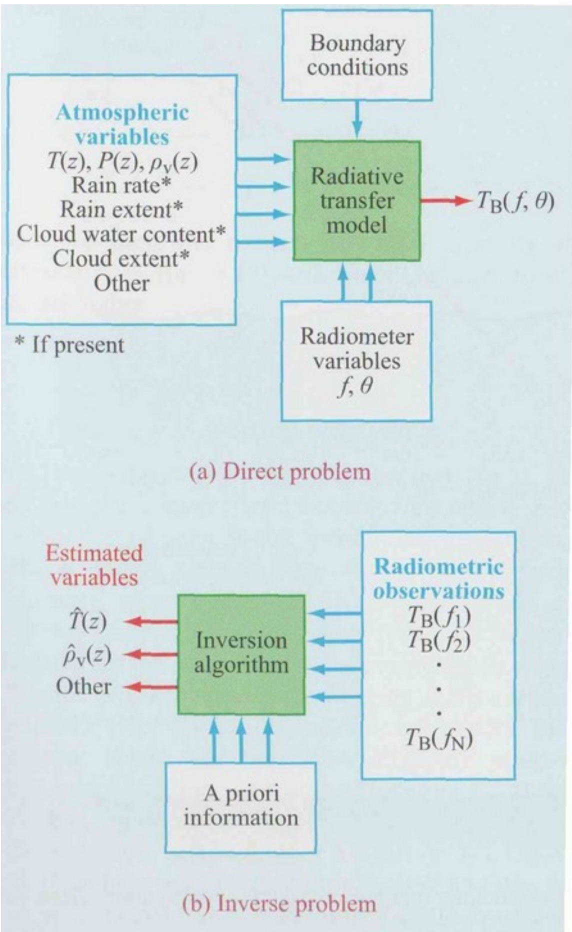
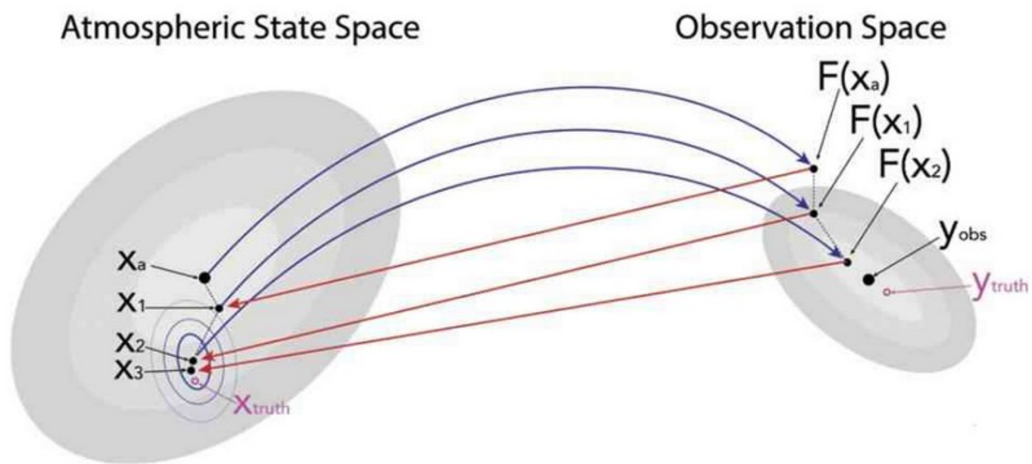


Figure 9-2: Elements of the (a) direct and (b) inverse problems in atmospheric remote sensing.

From *



Estimated Atmospheric state:

$$\mathbf{x}_{i+1} = \mathbf{x}_a + (\mathbf{S}_a^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{S}_e^{-1}\mathbf{K}_i)^{-1}\,\mathbf{K}_i^{\mathrm{T}}\mathbf{S}_e^{-1}[\mathbf{y} - \underbrace{F(\mathbf{x}_i,\mathbf{b}) + \mathbf{K}_i}_{\text{Forward model}}(\mathbf{x}_i - \mathbf{x}_a)],$$

Convergence criteria:

$$(\mathbf{x}_i - \mathbf{x}_{i+1})^{\mathrm{T}}\,\mathbf{S}_i^{-1}(\mathbf{x}_i - \mathbf{x}_{i+1}) \ll \mathrm{length}(\mathbf{x})$$

Uncertainty of the estimation:

$$\mathbf{S}_i = (\mathbf{S}_i^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{S}_e^{-1}\mathbf{K}_i)^{-1}.$$

Scheme and equations from [1]

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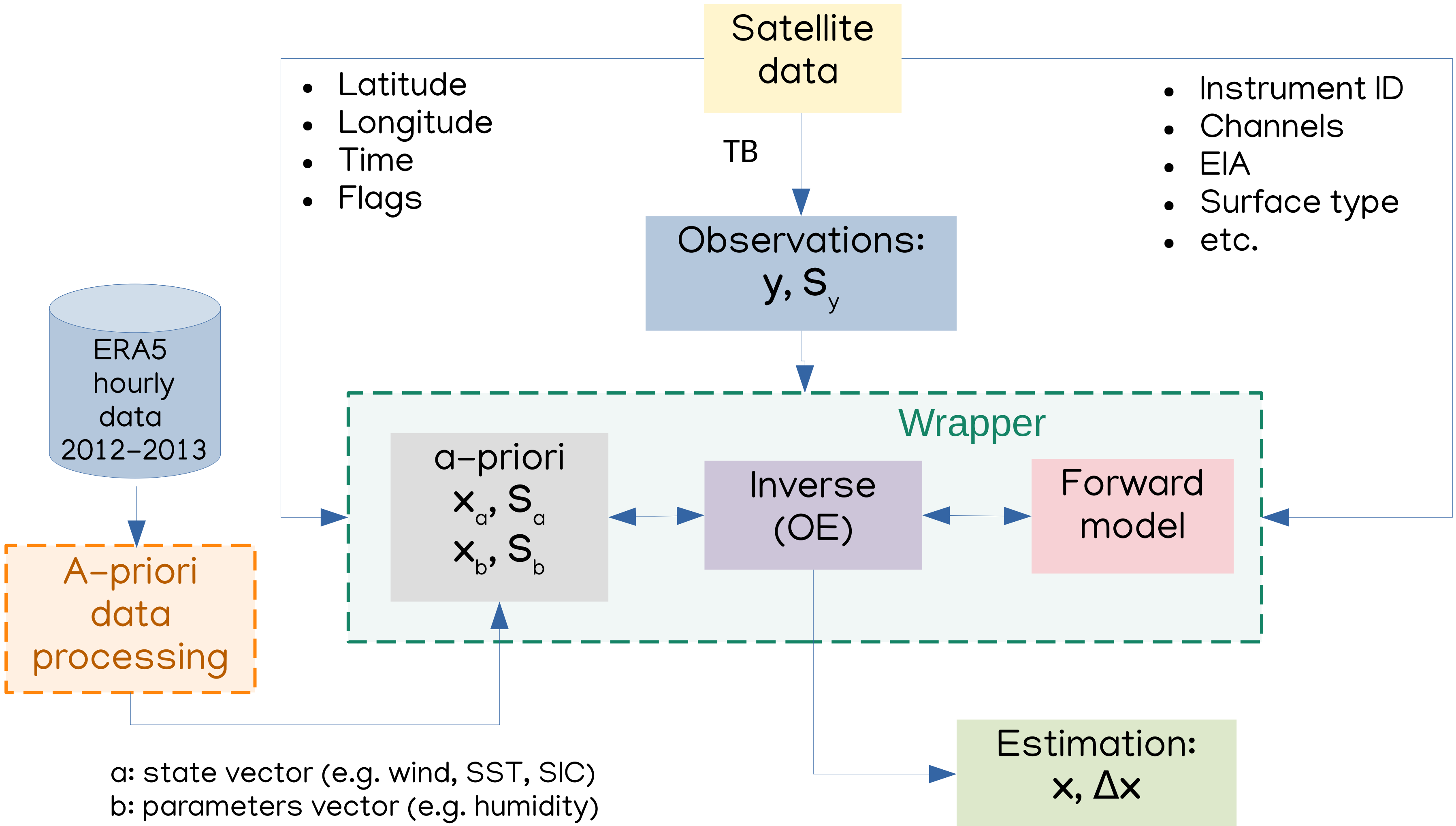
* F. Ulaby, D. Long, "Microwave Radar and Radiometric Remote Sensing", The University of Michigan Press, 2014.

The OE pipeline:



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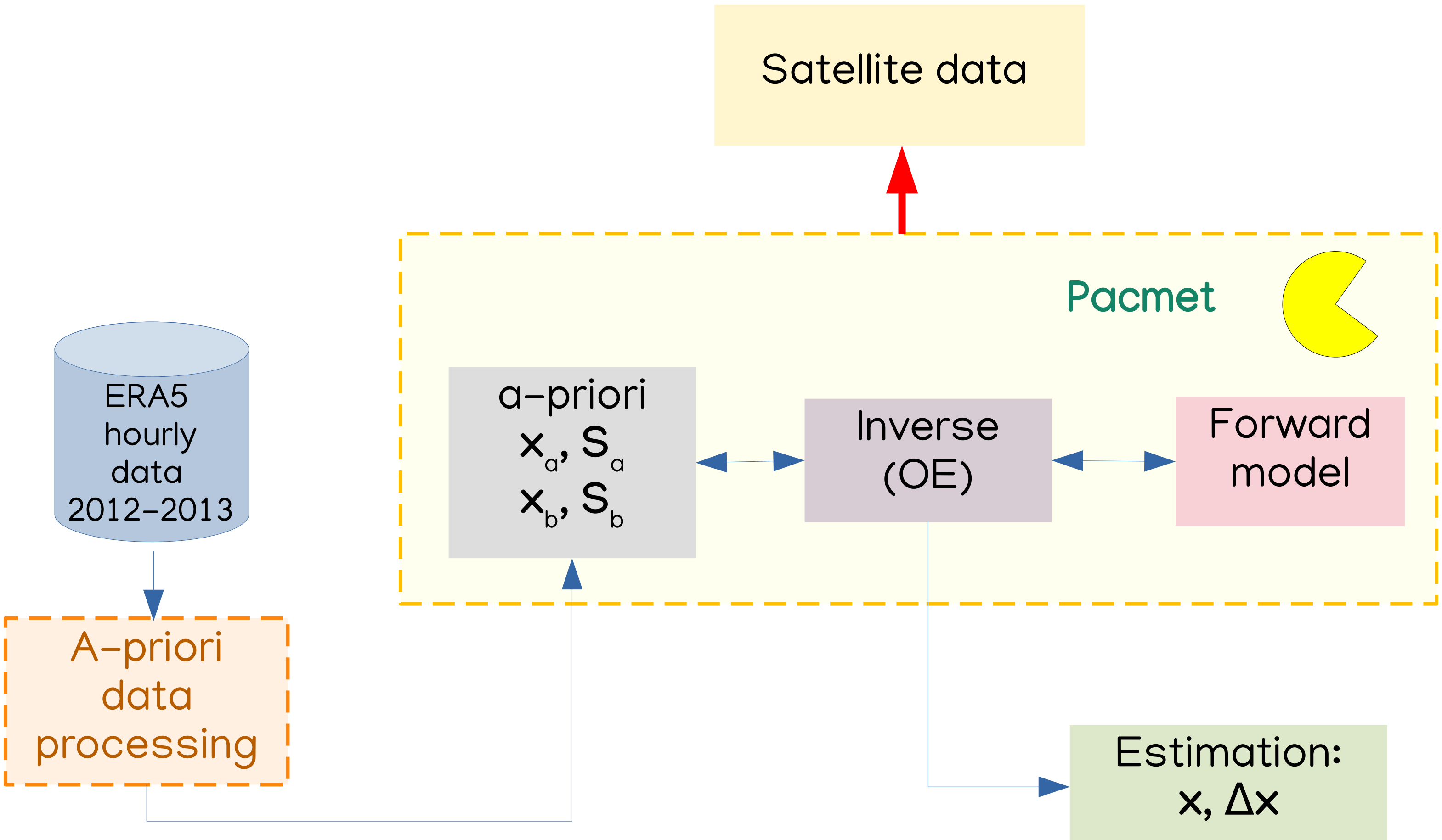

a: state vector (e.g. wind, SST, SIC)
b: parameters vector (e.g. humidity)

How: Load in lazy format

```
Dataset = xr.open_dataset('today.nc').chunk({"time": chunk_size_time,
                                             "scene_across_track": chunk_size_s_a_t})
```

xarray.Dataset

► Dimensions: (**time**: 45505, **scene_across_track**: 90, **scene_channel**: 5)

▼ Coordinates:

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*TB from CMSAF: https://wui.cmsaf.eu/safira/action/viewDoiDetails?acronym=FCDR_MWI_V003

How: what is this?

```
Dataset = xr.open_dataset('today.nc').chunk({"time": chunk_size_time,
                                             "scene_across_track": chunk_size_s_a_t})
```

xarray.Dataset

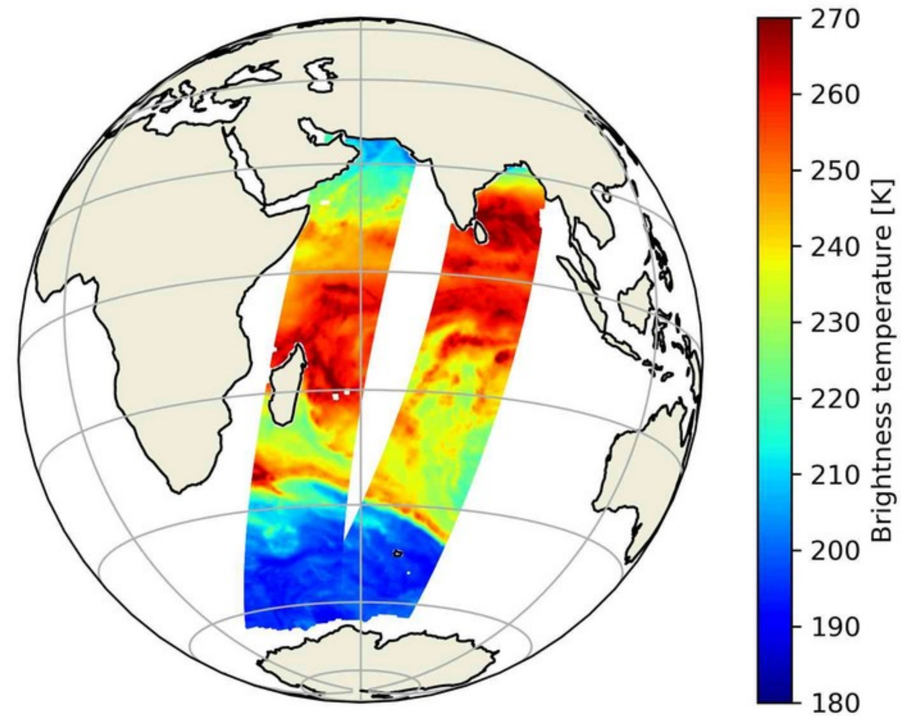
► Dimensions: (**time**: 45505, **scene_across_track**

▼ Coordinates:

scene_across_…	(scene_across_track)
scene_channel	(scene_channel)
time	(time)

▼ Data variables:

lat	(time, scene_across_track)
lon	(time, scene_across_track)
eia	(time, scene_across_track)
sft	(time, scene_across_track)
tb	(time, scene_across_track, scene_c
global_channel…	(scene_channel)
channel_uncert…	(scene_channel)



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*TB from CMSAF: https://wui.cmsaf.eu/safira/action/viewDoiDetails?acronym=FCDR_MWI_V003

How: chunks and tasks, simple

Chunks of data:

tb (time, scene_across_track, scene_channel) float32 dask.array<chun...

	Array	Chunk
Bytes	58.01 kiB	14.94 kiB
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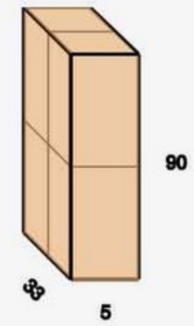
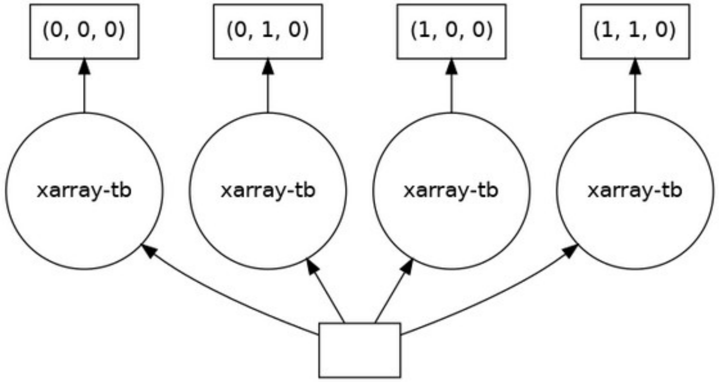


Graph of tasks:



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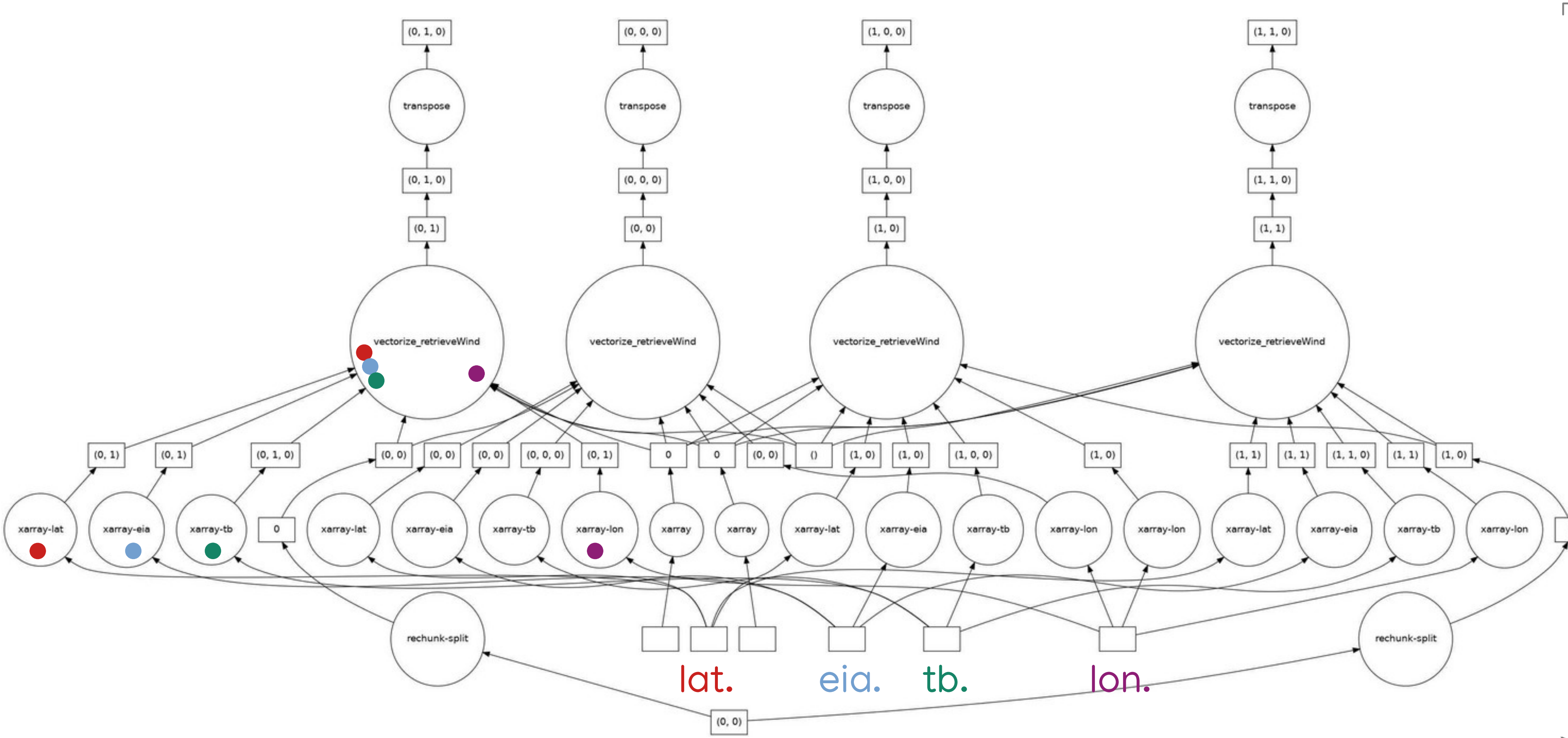
How: retrieval graph of tasks



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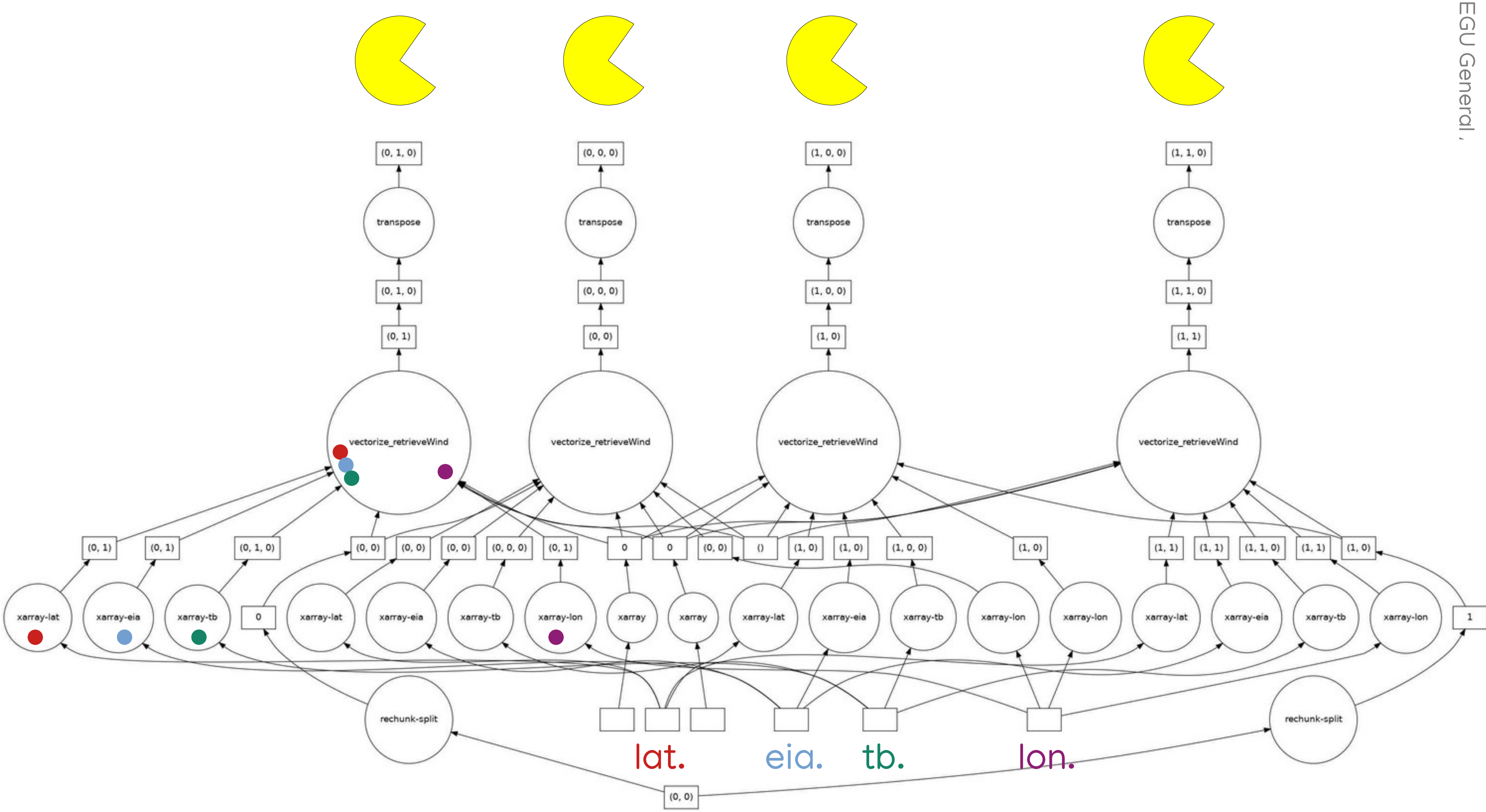
How: tasks scheduled among workers



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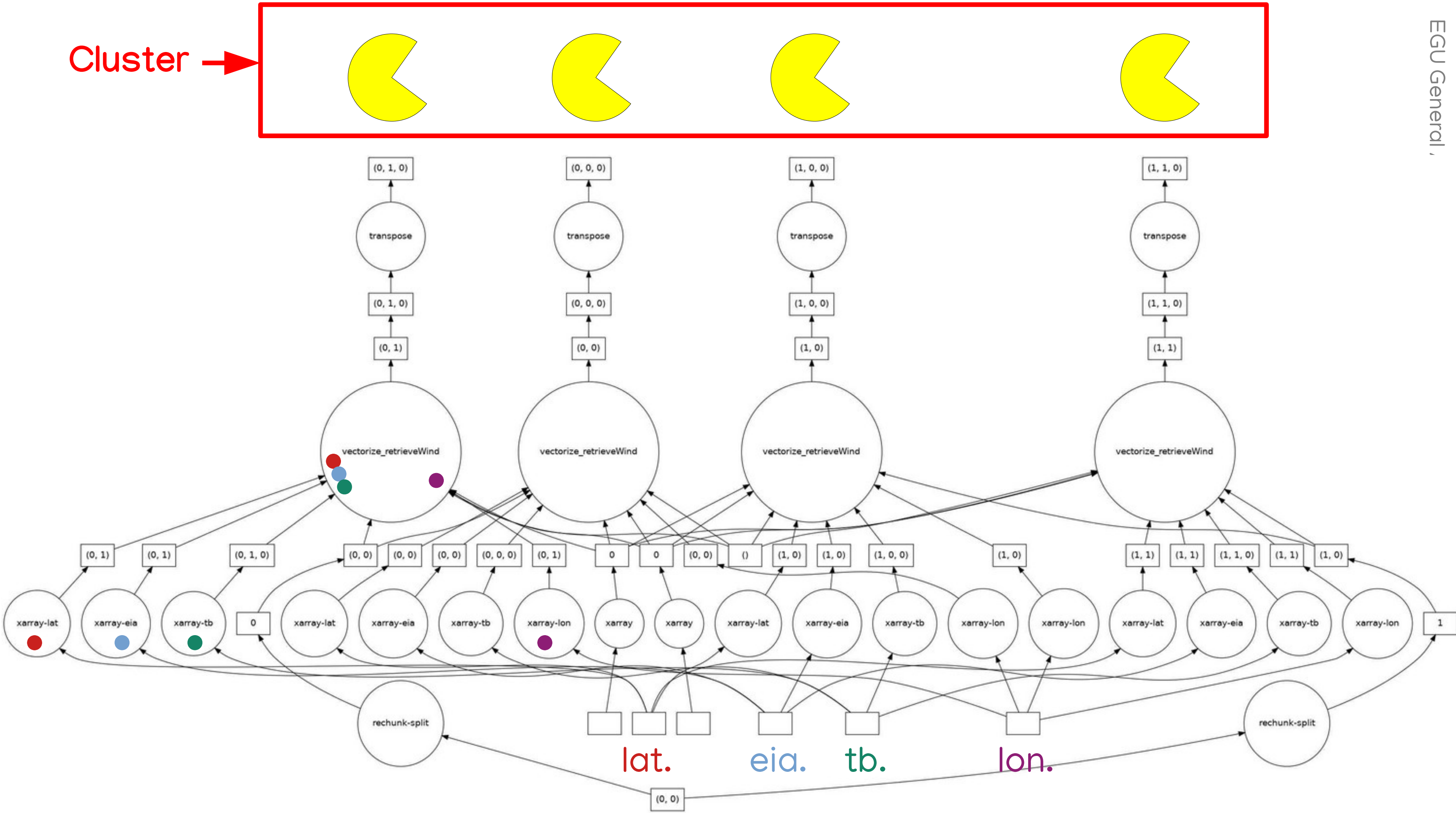

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How: Computation clusters

- Dask offers a broad spectrum of cluster managers in its API:
  - LocalCluster (i.e. your computer with all its workers)
  - SSHCluster (i.e. a cluster of computers connected through ssh)
  - CloudProvider (i.e. leveraging cloud native API's)
    - FargateCluster (AWS)
    - Elastic Compute Cloud, EC2 (AWS)
    - Elastic Container Service (AWS)
    - DropletCluster (DigitalOcean)
    - GCPCluster (Google Cloud)
    - AzureVMCluster (Microsoft Azure)

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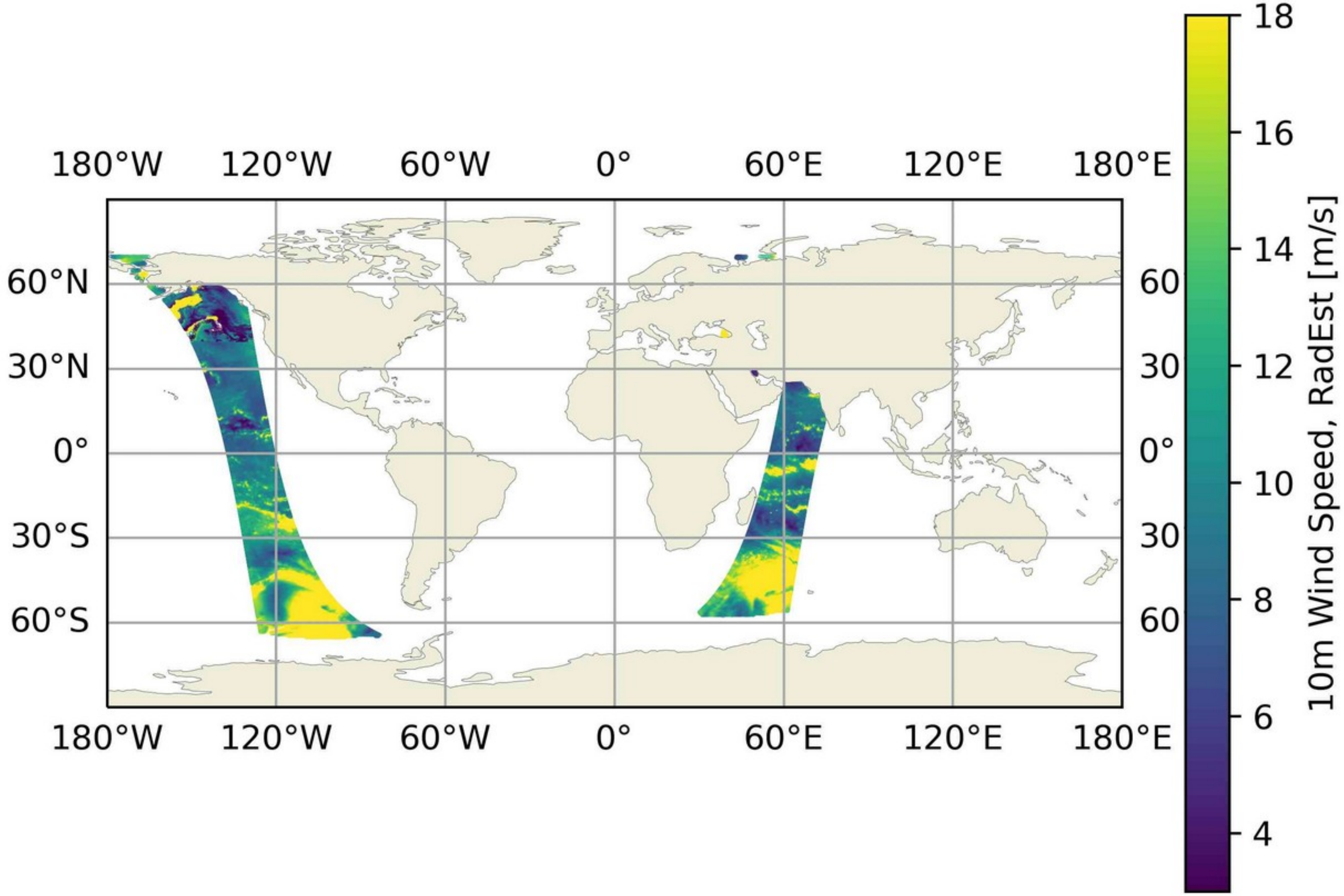
Some results:

- Wind retrievals using CMSAF SSMIS (F16) Temperature Brightness (2 hours in September 2014).
- For testing purposes we use a-priori data computed using ERA5:
  - Mean (x_a , x_b): Climatological mean (2012-2013)
  - Covariance (S_a , S_b): natural variability in the dataset*.

* This is not representative of the background error covariance, which turns out to be a whole are of research on its own, but it gives a good starting point to test.

Some results: retrieved wind speed x_{op}



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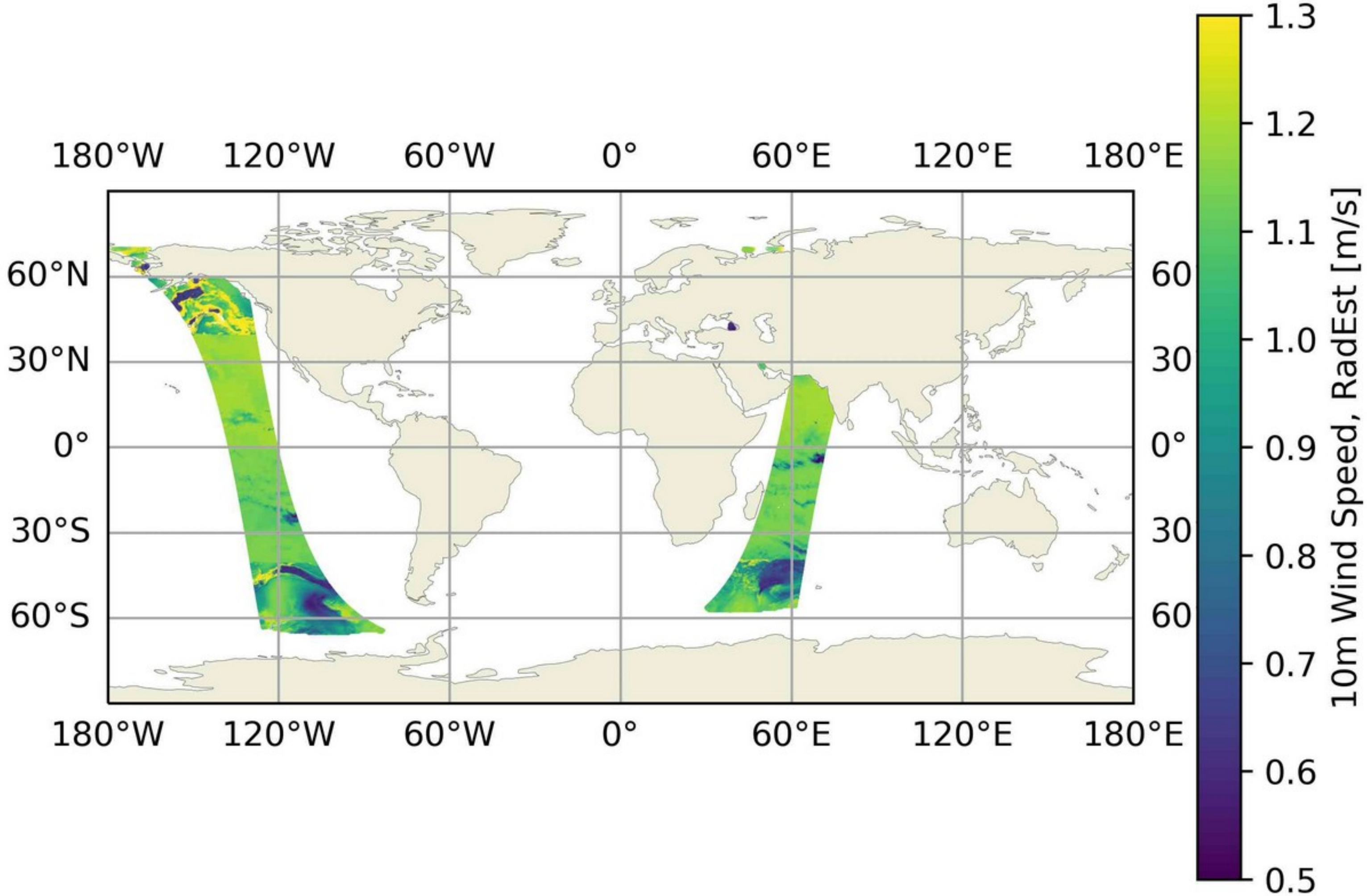
Some results: uncertainty of retrieval x_{err}



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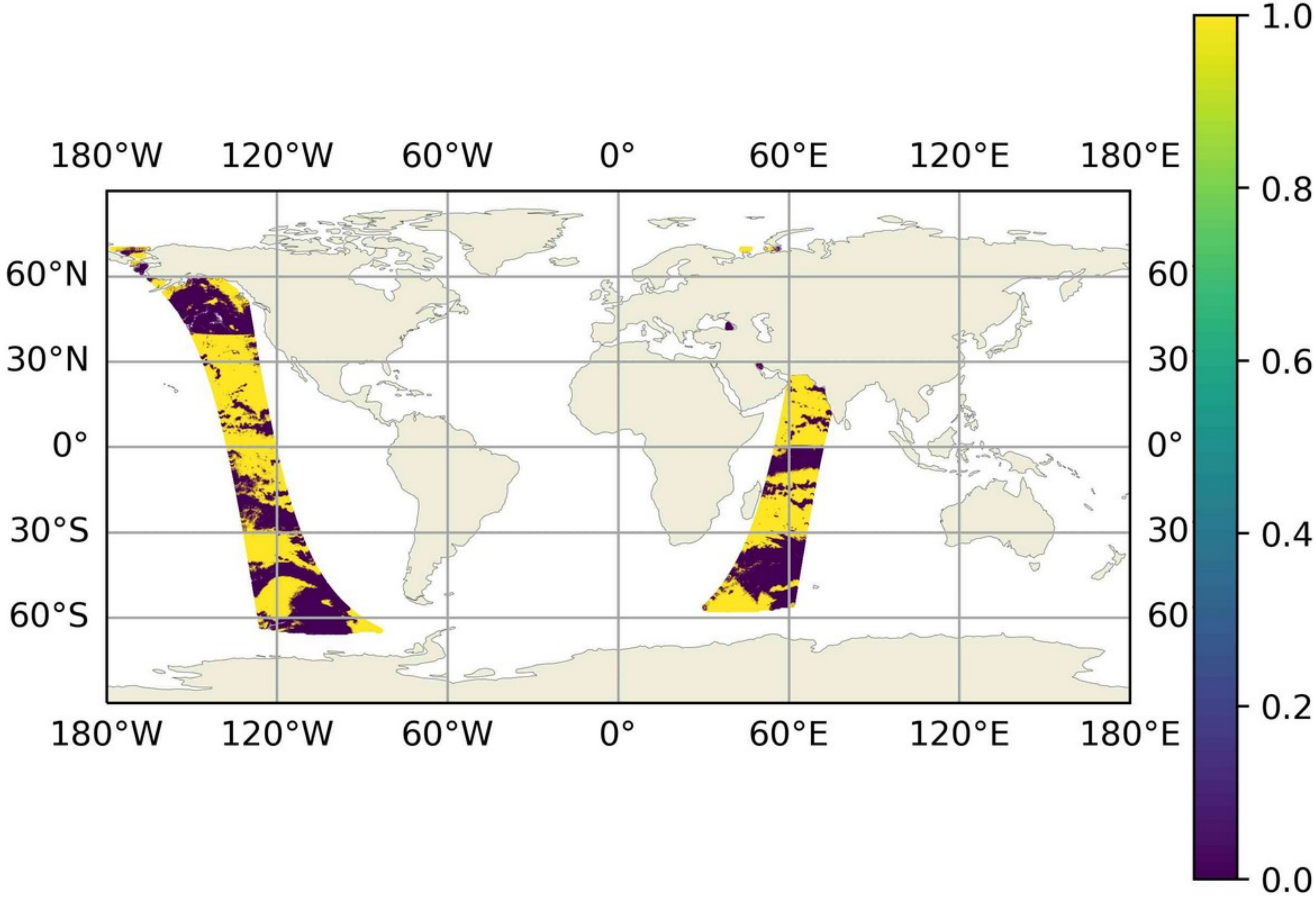
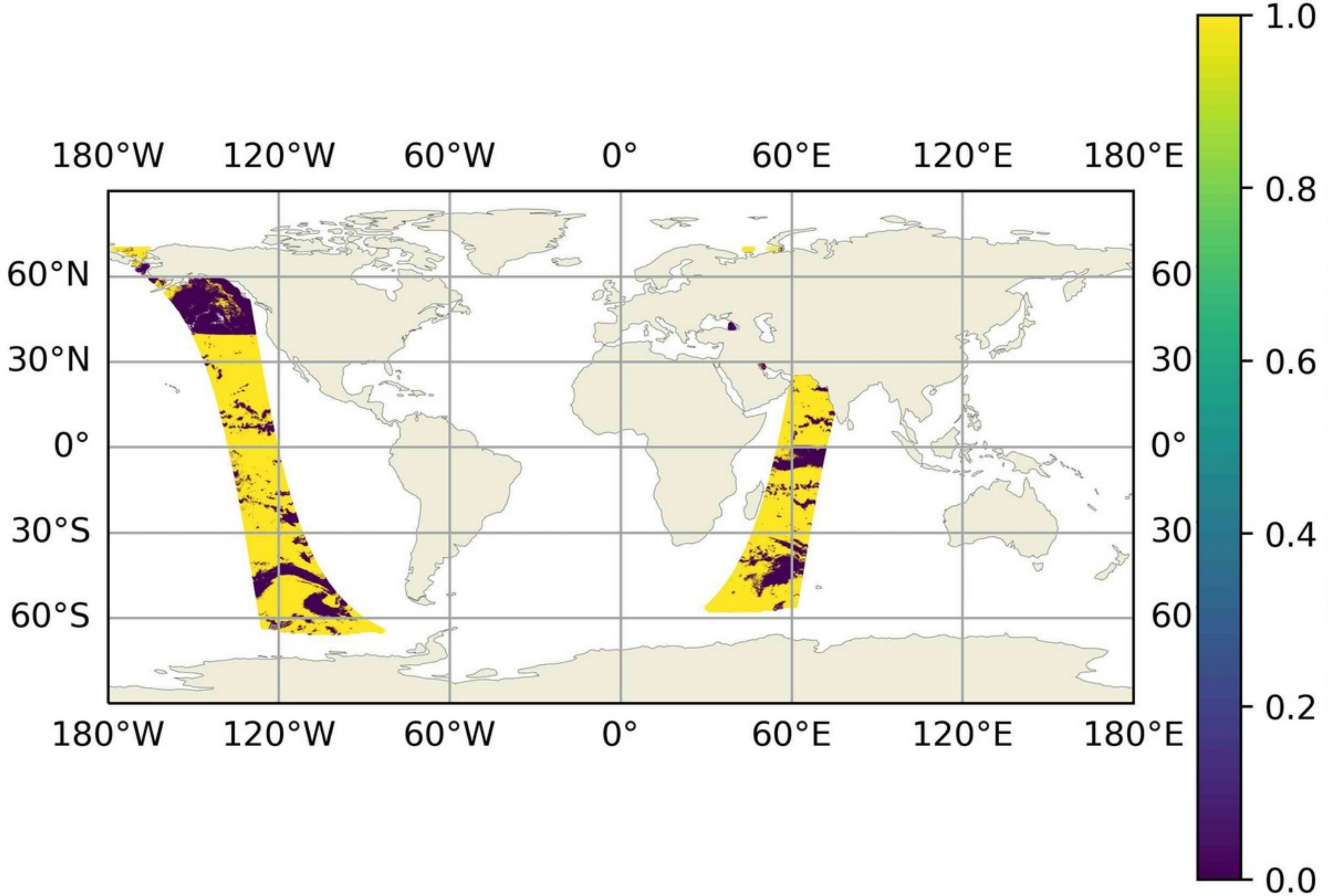
Statistical tests suite

- It is desirable to have at hand tools to evaluate the quality of the retrievals.
- Rodgers proposed a few diagnostics based on χ^2 testing (e.g. test whether or not a particular vector belongs to a given Gaussian distribution):
  - T0, y_optimal vs Obs.: $(y_{op} - y_{obs})$
  - T1, Obs. vs y_prior: $(y_{obs} - y_a)$
  - T2, y_optimal vs y_prior: $(y_{op} - y_a)$
  - T3, x_optimal vs x_prior: $(x_{op} - x_a)$

Some results: test ($y_{op} - y_{obs}$)



Some results: test ($y_{obs} - y_a$)



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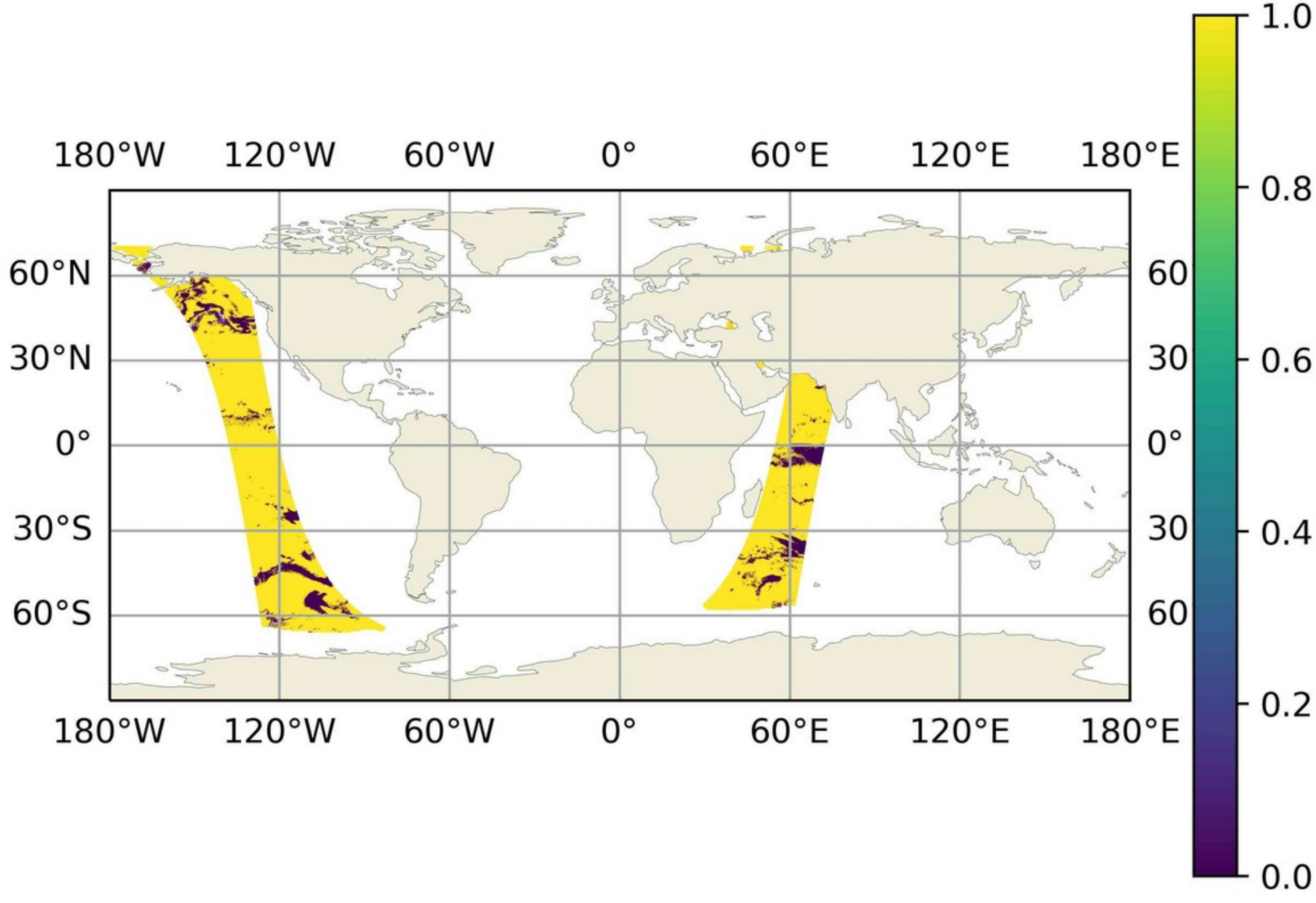
Some results: test (y_{op} – y_a)



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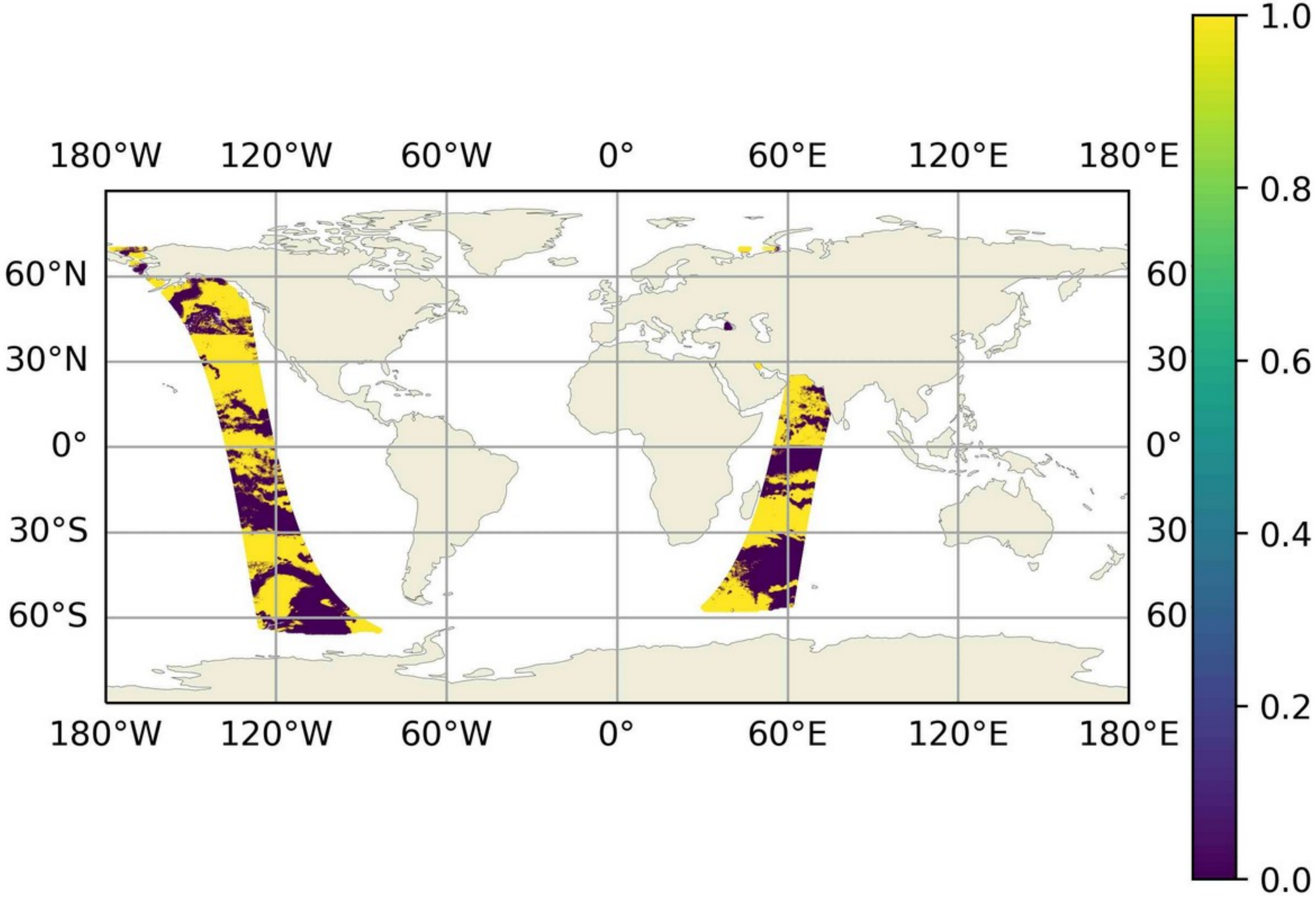
Some results: test ($x_{op} - x_a$)



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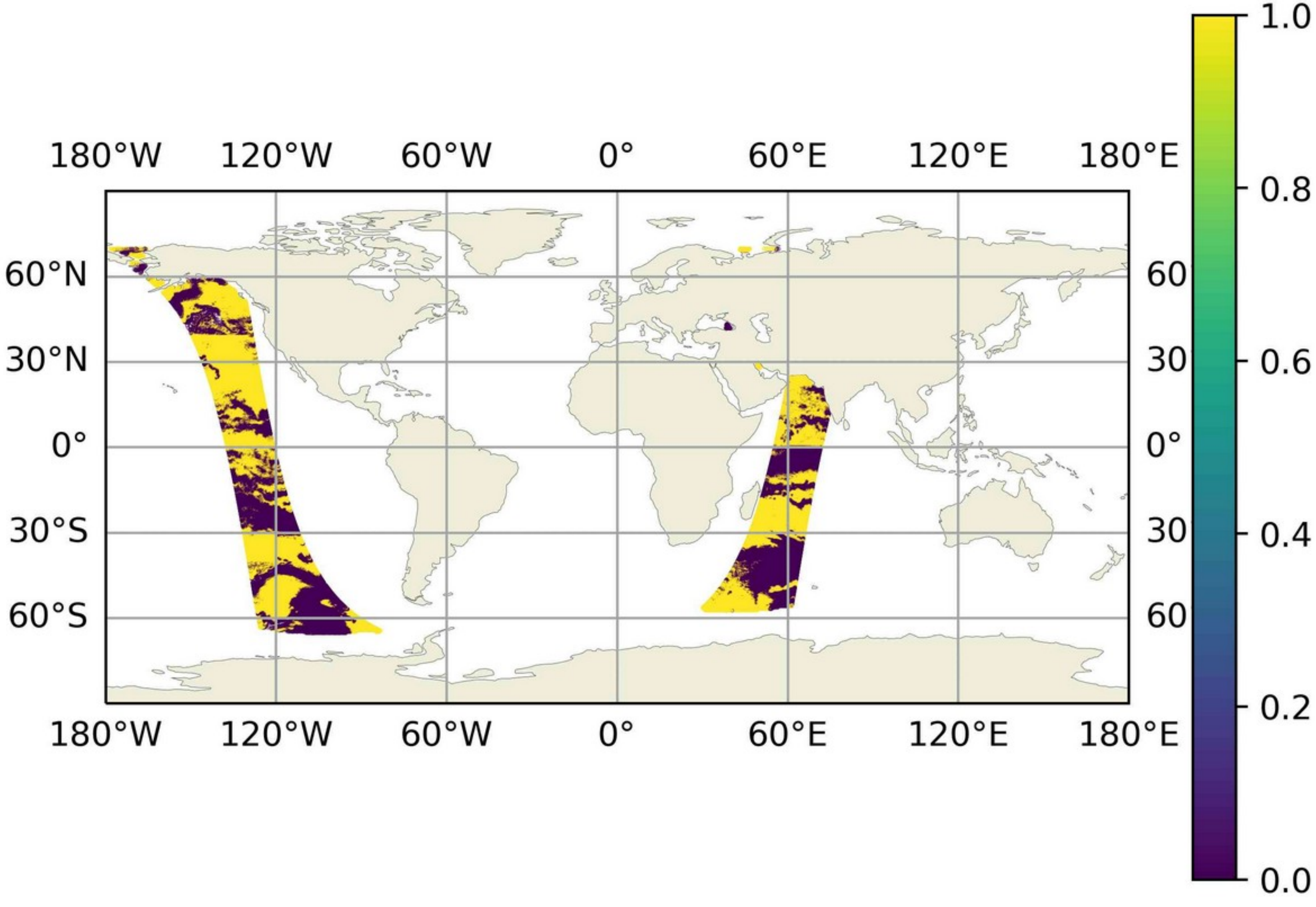

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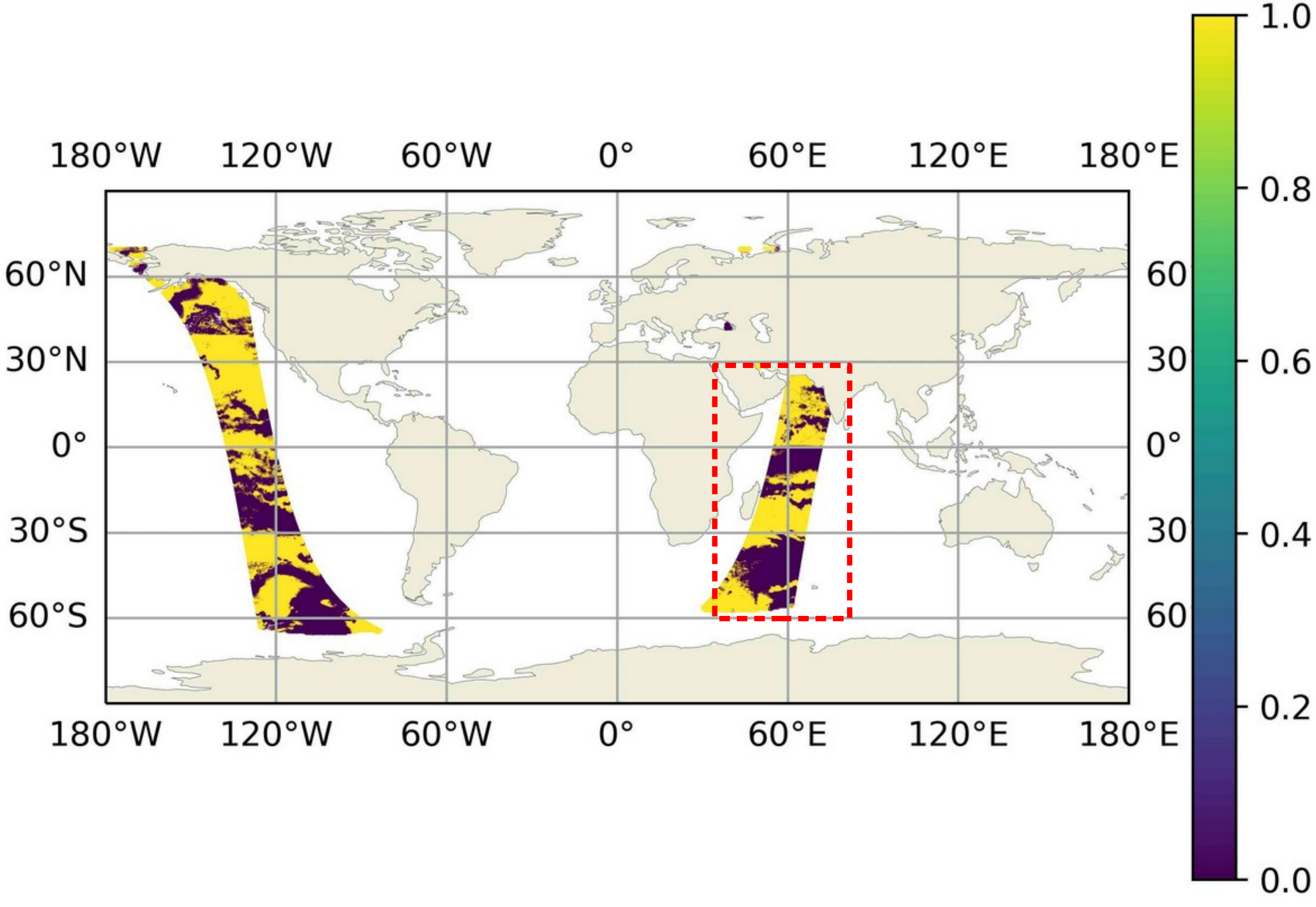
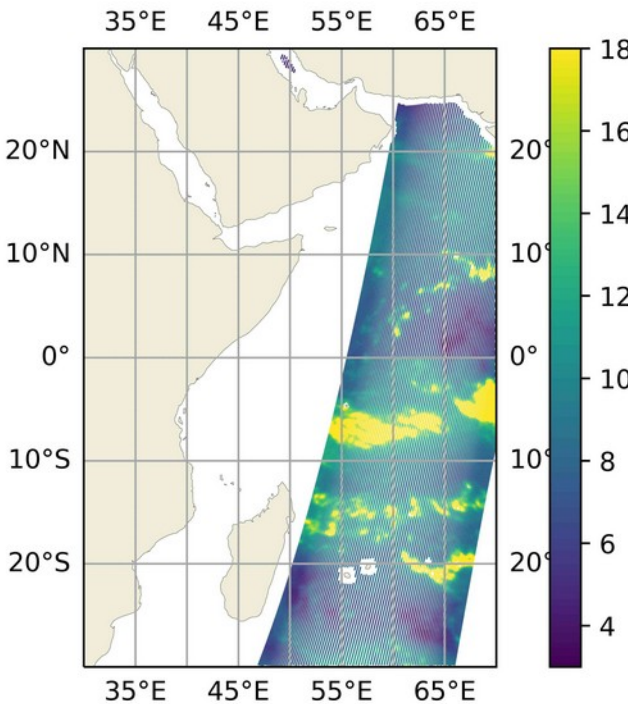
Some results: test ($x_{op} - x_a$)

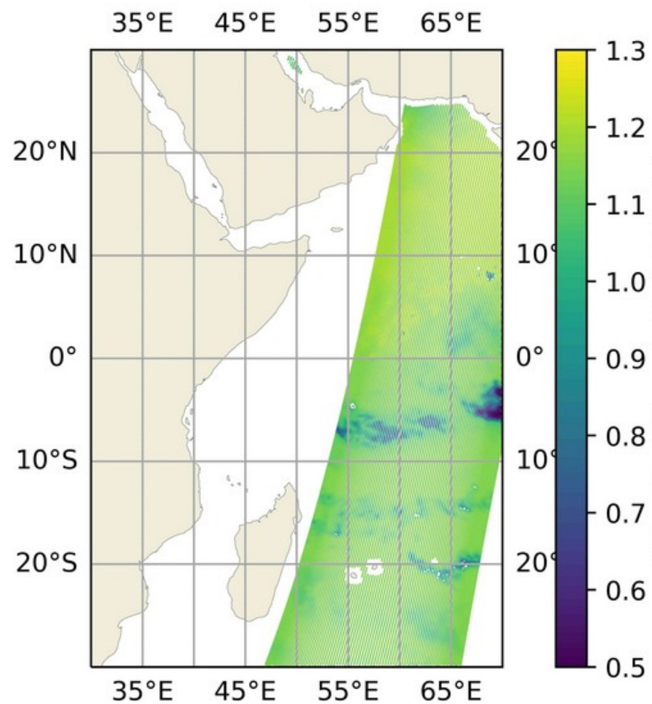


Some results: All pass

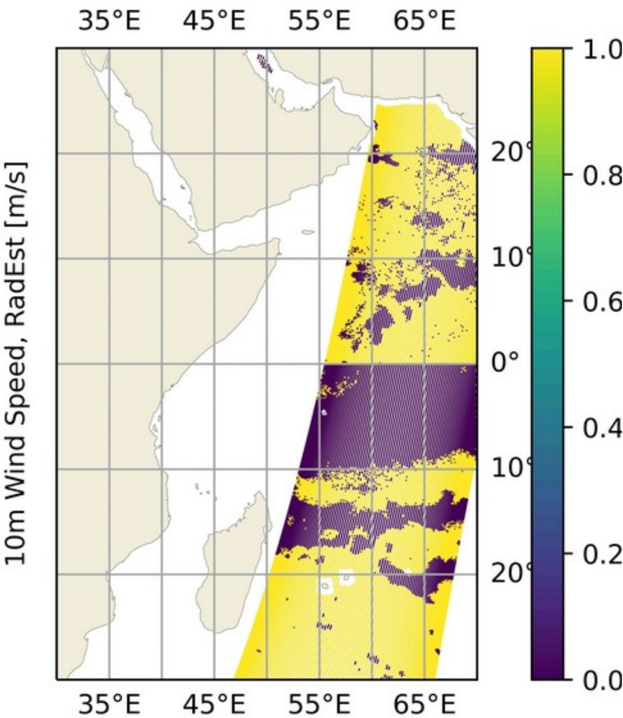
Wind speed



Wind uncertainty

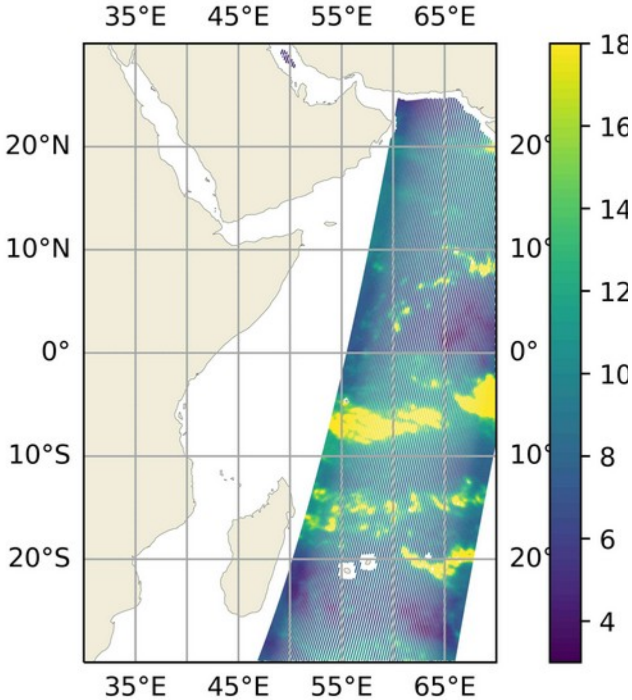


T0 & T1 & T2 & T3

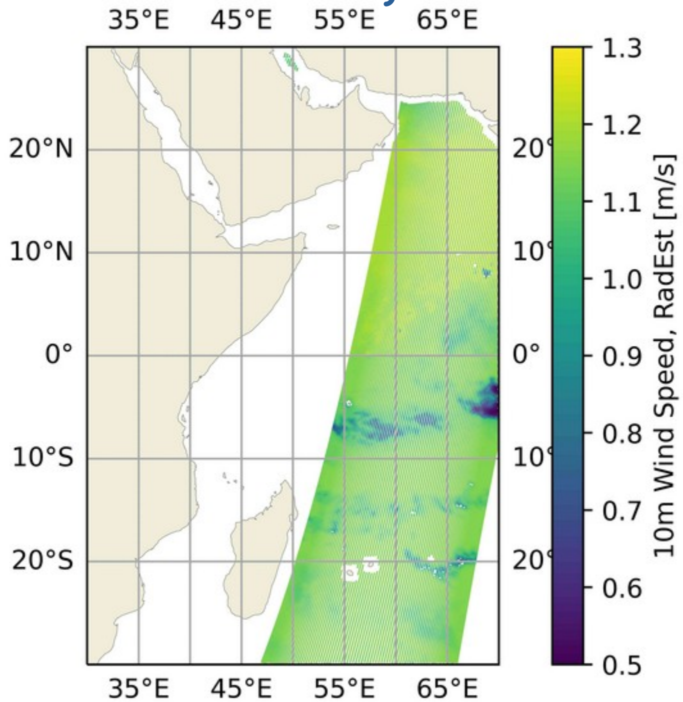


Some results: All pass

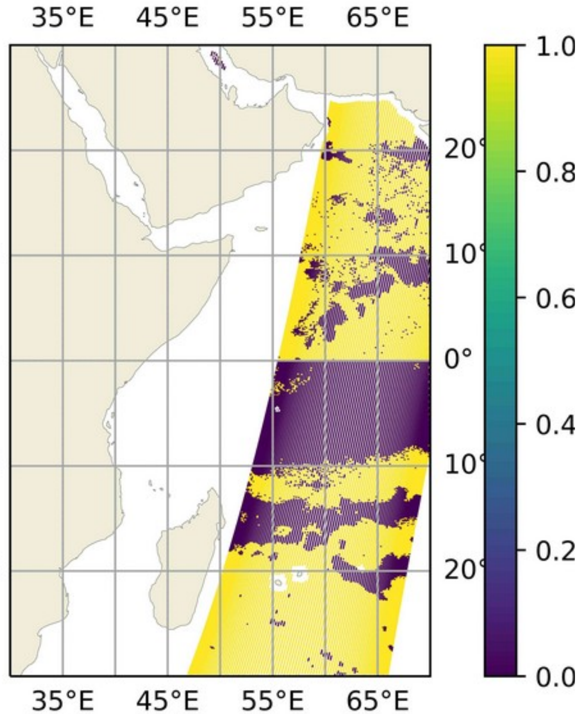
Wind speed



Wind uncertainty



T0 & T1 & T2 & T3



T0, y_optimal vs Obs.: $(y_{op} - y_{obs})$

T1, Obs. vs y_prior: $(y_{obs} - y_a)$

T2, y_optimal vs y_prior: $(y_{op} - y_a)$

T3, x_optimal vs x_prior: $(x_{op} - x_a)$

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Work in progress:

- Containerization:
  - Pack the whole "app" in a deploy-friendly container > Docker containers.
- Cloud resources:
  - What and how to use > AWS.
- A-priori error covariances:
  - Properly estimate the error variability within the ERA5 dataset (e.g. forecast model error).
- Documentation:
  - Reports
  - Markdown (for nicely documented code).

To conclude:

- A classical physical retrievals scheme was re-cast using modern Python.
- The Pangeo stack is being actively used in order to facilitate the connection between low level algorithms and high level interfaces.
- The Pangeo stack provides tools that can be integrated in a satellite observations processing pipeline and opens doors to high performance deployment in a straightforward manner.

References

[1] M. Maahn et al, “Optimal Estimation Retrievals and Their Uncertainties What Every Atmospheric Scientist Should Know”, BAMS, Vol. 101, Issue 9, Sept. 2020

[2] C. D. Rodgers, “Inverse Methods for Atmospheric Sounding, Theory and Practice”, World Scientific Pub., 2000.

Thanks!

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Questions?

mario.echeverribautista@knmi.nl

https://github.com/deweatherman

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