# **DESTINATION EARTH**

# **AQUA**

THE QUALITY ASSESSMENT TOOL FOR THE **CLIMATE DIGITAL TWIN** 

Silvia Caprioli and the AQUA team



3rd Destination Earth User eXchange, Darmstadt, 15 October 2024























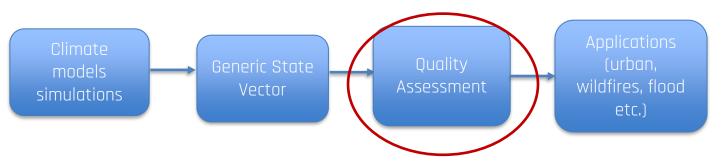
# **Destination Earth: The Climate Digital Twin**

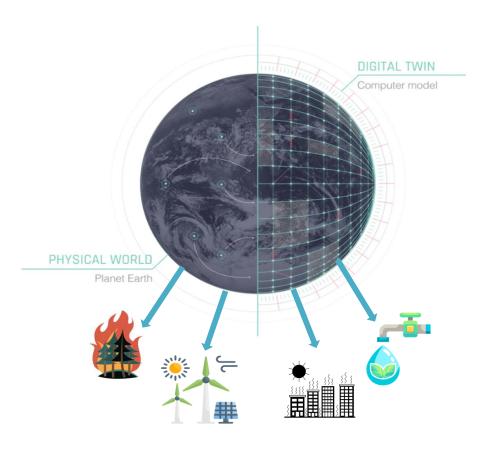
### The Climate Digital Twin

#### **Key Features**:

- Global climate simulations at **km-scale horizontal resolution**
- User-driven approach focused on **user interactivity**
- **Streaming framework** from climate model output to impact sectors
- Quality assessment and uncertainty quantification based on observations

### **AQUA Application for Quality Assessment**



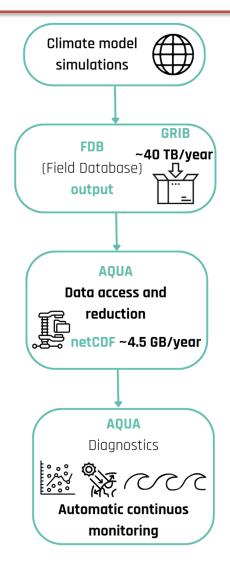




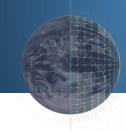
# Model evaluation in the Climate DT: The need for AQUA

Many tools are available for climate model analysis (ESMValTool, E3SM, CMEC...). However, Climate DT simulations presents specific challenges:

- Global climate simulations at **unprecedented horizontal** (5 km atm and ocean) and **temporal resolution** (1 hour)
- **Amount of data** for a single simulation is critically high: 40 TB per simulated year (at the moment: 5.7 PB of Climate DT data in total)
- Data access through FDB, with data both locally on HPC and remote on Data Bridge/Data Lake
- Flexible to support the introduction of a **streaming framework** for **continuous and automatic monitoring** of model output
- Deployment and portability on multiple European **pre-exascale supercomputers** (LUMI, Levante, MareNostrum5 etc.)



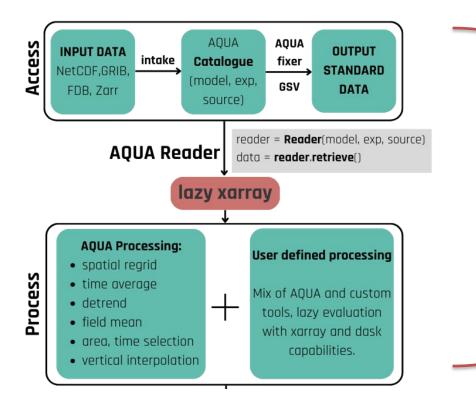




## The Philosophy of AQUA

AQUA provides a framework to access, process and analyze large volumes of climate data

- making data access simple (two lines of code to get a dask-enabled xarray)
- dealing with all the technicalities (grid weights, FDB requests, different variable names and units, ecCodes versions) behind the scenes.



Python3 library package based on xarray, dask, CDO and intake

**Technical details are hidden** simple user experience

Lazy access to all data (parallel dask enabled) including FDB

**Modular structure** seamless integration between core functions

**Fast regrid capabilities** based on precomputed weights

CI/CD on every new code addition with around 75% code coverage

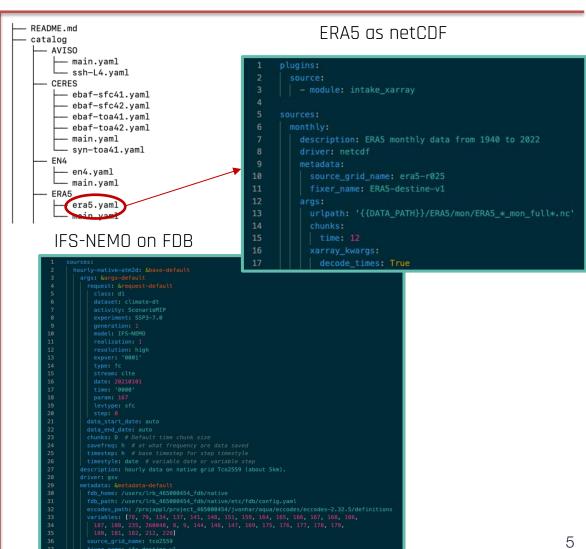
for the framework





## **AQUA core concepts: the Catalog**

- Folder containing paths and technical details of all the sources that the user may want to access (models and observational datasets)
- Built on **intake** package
- **3 level hierarchy: model** (e.g. IFS, ERA5) **experiment** (e.g. historical, scenario) **source** (e.g. hourly-native, monthly-r100)
- **FDB GRIB** data as well as **NetCDF**. **Zarr** and other formats can be used with small effort
- Machine independent







### **AQUA** core concepts: the Reader

Once a catalog is added the user can retrieve the dataset with two lines of code!



```
from aqua import Reader
                        reader = Reader(model='IFS-NEMO', exp='historical-1990',
This is a lazy dask array!
                        source='hourly-native-atm2d', regrid='r100')
                      ★data = reader.retrieve()
```

### **Fixing**

- Data are automatically retrieved in a **common metadata format** (GRIB standard)
- Fixes are defined when creating a catalog source and then automatically enabled when data are retrieved

```
IFS
                           GSV
                    mtpr (kg m^{-2}s^{-1})
tp (m)
```

YAML file with **fixer\_name** that can be applied to multiple models/exps/sources

```
data model: False
ifs-destine-v1:
   data_model: ifs
   deltat: 3600
   delete: [tprate]
      # Derive precipitation from TP and drop tprate
                                                                                    valid max: 0
       mtpr: # https://codes.ecmwf.int/grib/param-db/235055
                                                                                    positive down
           nanfirst: true
           source: tp
          grib: true
       # Evaporation and snowfall
       mer: # https://codes.ecmwf.int/grib/param-db/?id=235043
                                                                                    valid min: 0
           grib: true
          src units: m
                                                                                    valid max: 1400
           nanfirst: True # option to fix ifs bug in destine-v
       msr: # https://codes.ecmwf.int/grib/param-db/?id=235031
           source: sf
           arib: true
           src units: m
           nanfirst: True
           #units: kg m**-2 s**-1
       # Latent and sensible heat
       mslhf: # https://codes.ecmwf.int/grib/param-db/?id=2356
           source: slhf
           grib: true
          nanfirst: True
       msshf:
           source: sshf
           grib: true
           nanfirst: True
```



### **AQUA** core concepts: the Reader

Once a catalog is added the user can retrieve the dataset with two lines of code!



```
from aqua import Reader
                                                                                                        Prepare for regrid
                         reader = Reader(model='IFS-NEMO', exp='historical-1990',
                                                                                                        to 1° deg resolution
This is a lazy dask array!
                         source='hourly-native-atm2d', regrid='r100')
                        →data = reader.retrieve()
                         data regridded = reader.regrid(data)
                                                                                                          Actual regrid
```

### Regridding

AQUA provides functions to interpolate and regrid data to match the spatial resolution of different datasets.

- Based on smmregrid package which operates sparse matrix computation based on pre-computed weights.
- Working on both native and **HealPix grids**
- Grids are defined in yaml file in AQUA and weights are evaluated with CDO only once.

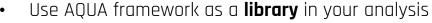


```
intained? yes () Mamba PyTest passing coverage 88% pypl package 0.0.6
                                                       smmregrid
  vert_coord: ["2d"]
                                                        A compact regridder using sparse matrix multiplication
  vert_coord: ["depth"]
                                                        This repository represents a modification of the regridding routines in climtas by Scott Wales, which already
                                                        implements efficiently this idea and has no other significant dependencies. The regridder uses efficiently spars
  space_coord: [lon, lat]
                                                        matrix multiplication with dask + some manipulation of the coordinates
r050: r720x360
r100: r360x180
  space_coord: ["ncells"]
  vert coord: ["2d"]
         '{{ grids }}/HealPix/hpz5 nested atm.nc'
  space_coord: ["ncells"]
         '{{ grids }}/HealPix/hpz7 nested atm.nc
```



# **AQUA** processing

**AQUA** core classes and functions can be integrated in any analysis



- Use available AQUA diagnostics
- Build your own AQUA diagnostic

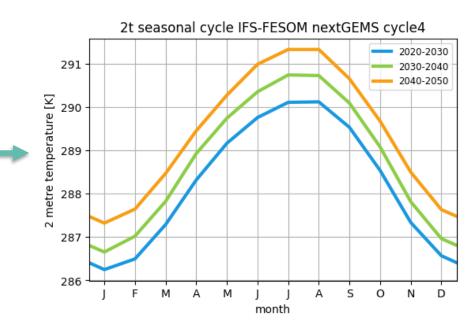
#### Simple example of custom analysis

#### Custom processing for a seasonal cycle

```
from aqua import Reader
reader = Reader(model='IFS-FESOM', exp='ssp370-ng4', source='lra-r100-monthly')
data 20 30 = reader.retrieve(var='2t', startdate='2020', enddate='2030')
cycle 20 30 = data 20 30['2t'].aqua.fldmean().groupby('time.month').mean('time')
```

#### Graphic utilities for a custom plot

```
from aqua.graphics import plot seasonalcycle
plot_seasonalcycle(data=[cycle_20_30, cycle_30_40],cycle_40_50], data_labels=['2020-
2030', '2030-2040', '2040-2050'], title='2t seasonal cycle IFS-FESOM nextGEMS
cycle4')
```







## The diagnostics suite

#### State-of-the-art

Provide general performance evaluation of the models and identification of biases and drifts.

Run on **low-resolution** data (daily/monthly, 1-deg)

- Performance indices: evaluation of model biases compared with CMIP6
- Timeseries and biases: timeseries of temperature, precipitation etc. 2d biases
- Radiation budget: model radiative budget imbalance
- Sea ice extent: seasonal cycles of sea ice extent in specific regions
- Teleconnection indices: NAO and ENSO indices and their pattern correlations
- Ocean circulation evaluation: evaluation of anomalies of oceanic variables. (temperature, salinity, density, mixed layer depth etc.)

#### **Frontier**

Provide insights into physical/dynamical processes not yet explored in classical climate simulations

Run on high-resolution data (hourly, km-scale)

- Sea Surface Height variability: to evaluate surface ocean dynamics
- **Tropical Rainfall:** analysis of tropical precipitation extremes
- Tropical cyclones detection, tracking and zoom-in: detection and tracking of tropical cyclones. Set of variables (precipitation, wind etc...) around the Tc's center at high resolution







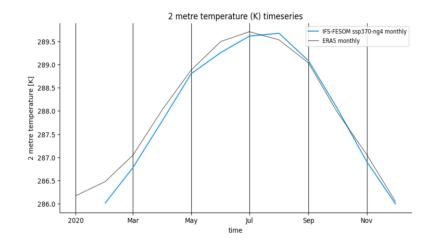
# Running diagnostics in AQUA

Diagnostics in AQUA are organized in a **modular structure** as separate Python classes/functions

### Use directly a diagnostics' function in a Jupyter notebook

```
from global_time_series import Timeseries
4.3s
```

```
ts = Timeseries(var='2t', models='IFS-FESOM', exps='ssp370-nq4', sources='lra-r100-monthly',
                startdate='2020-01-01', enddate='2020-12-31',
                std_startdate='2020-01-01', std_enddate='2020-12-31',
                loglevel='INFO')
 0.0s
```



- Run them independently and in parallel
- Easy to add custom diagnostics

#### Run a single diagnostic with a cli

### series/cli> python cli\_global\_time\_series.py -c config\_time\_series\_atm.yaml

```
diagnostics > global_time_series > cli > ! config_time_series_atm.yaml
      # The first model in this block can be overridden
     # in the command line by using:
      # --model, --exp, --source, --outputdir
        - model: 'IFS-NEMO
          exp: 'ssp370'
          source: 'lra-r100-monthly'
      outputdir: "./"
      # This is the list of variables that will be plotted as timeseries
      timeseries: ['2t', 'mtpr', 'mer', 'msl',
                   'tcc', 'lcc', 'mcc', 'hcc',
13
                   'mslhf', #Mean surface latent heat flux
14
                    'msshf', #Mean surface sensible heat flux
15
                    'msdwswrf', #Mean surface downward short-wave radiation flux
                    'msdwlwrf', #Mean surface downward long-wave radiation flux
                    'msnswrf', #Mean surface net short-wave radiation flux
                    'msnlwrf', #Mean surface net long-wave radiation flux
19
                    'mtnlwrf', #Mean top net long-wave radiation flux
                   'mtnswrf' #Mean top net short-wave radiation flux
21
22
      timeseries_formulae: ['mtnlwrf+mtnswrf']
23
24
      gregory:
        toa: ['mtnlwrf', 'mtnswrf']
       monthly: True
```

config file where the user can specify model, exp, source, variables, output dir etc.







## Running diagnostics in AQUA

Diagnostics in AQUA are organized in a **modular structure** as separate Python classes/functions



- Run them independently and in parallel
- Easy to add custom diagnostics

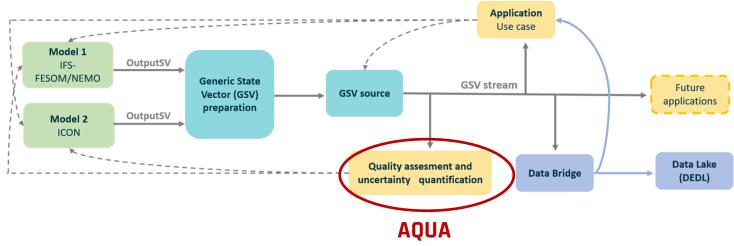
#### Run all the diagnostics for a complete analysis

#### 2024-04-04 14:34:11: Setting loglevel to WARNING 2024-04-04 14:34:11: Atmospheric model: IFS-NEMO 2024-04-04 14:34:11: Oceanic model: IFS-NEMO 2024-04-04 14:34:11: Experiment: historical-1990 2024-04-04 14:34:11: Source: lra-r100-monthly 2024-04-04 14:34:11: Machine: lumi 2024-04-04 14:34:11: Output directory: ./output 2024-04-04 14:34:11: Machine set to lumi in the config file 2024-04-04 14:34:11: Creating output directory //output 2024-04-04 14:34:11: Running setup checker 2024-04-04 14:35:25: Finished setup checker 2024-04-04 14:35:25: Running tropical\_rainfall 2024-04-04 14:35:25: Running seasonal\_cycles-2024-04-04 14:35:25: Running radiation 2024-04-04 14:35:25: Running teleconnections 2024-04-04 14:35:25: Running atmglobalmean 2024-04-04 14:35:25: Running global\_time\_series 2024-04-04 14:35:25: Running teleconnections nal as a climi 2024-04-04 14:35:26: Running ocean3d\_drift 2024-04-04 14:35:26: Running ocean3d\_circulation 2024-04-04 14:35:26: Running segice\_extention Jost von Hard 2024-04-04 14:35:26: Running seaice\_conc

### Real-time monitoring of ongoing simulations



Integration into the general Climate-DT **workflow** is in progress

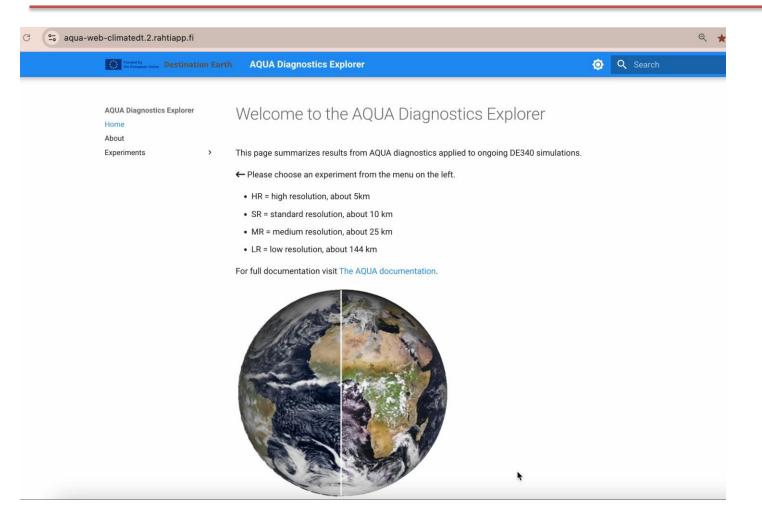








# Real time monitoring: the AQUA explorer



**Real-time monitoring** is already implemented for the running DestinE simulations through the AQUA explorer

Diagnostics are run <u>everyday on Climate DT runs</u> and all the results are published on a dedicated website.

Developed by AQUA using infrastructure by CSC

- Automatic experiment page generation
- Integrated and dynamical figure caption generation
- Single tab for each experiment
- It will be replaced by a dashboard



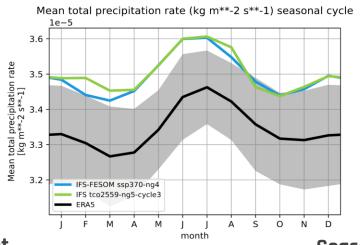


### **Example plots**

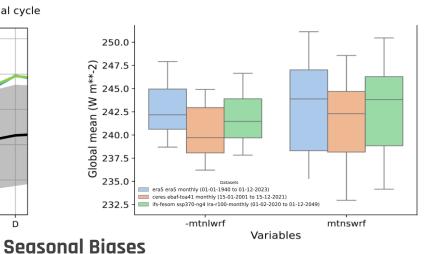
#### **Global timeseries**

#### 2 metre temperature (K) timeseries IFS-FESOM ssp370-ng4 monthly IFS-FESOM ssp370-ng4 annual 291 ERA5 monthly ERA5 annua 289 5 288 288 E 287 286 2020 2024 2028 2032 2036

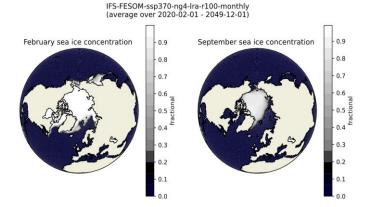
### **Seasonal Cycles**



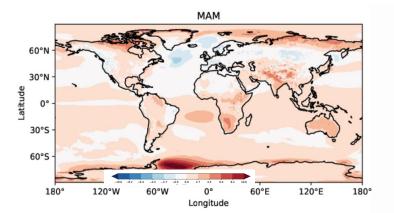
#### **Radiation budget**



#### Sea ice extent



#### Bias of 2t [K] (mean) from (2020-2-1 to 2049-12-1)



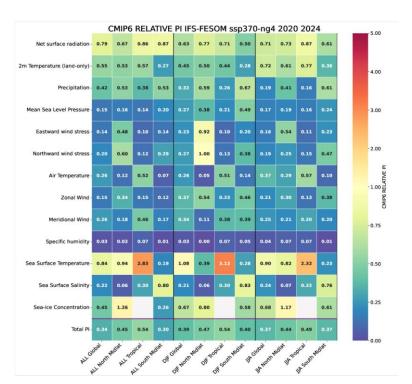




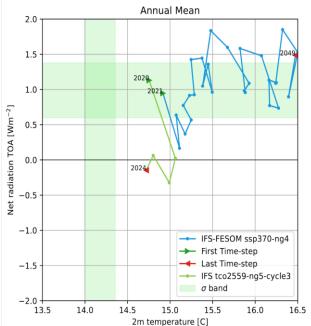


### **Example plots**

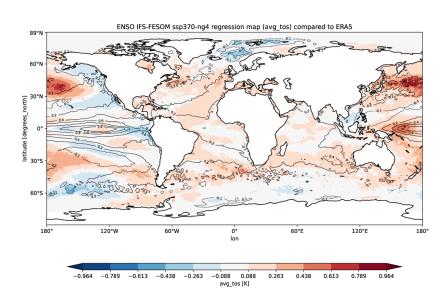
#### Performance indices



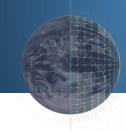
#### **Gregory plots**



#### Teleconnections maps







## **Development plans**

- Keep AQUA updated with respect with **changes in data portfolio** and eccodes versions, **HPC machines** and **Data Bridge** specifications for Climate DT purposes
- Transition toward **open source package** by refactoring the installation procedure (done) the diagnostics structure and the agua-analysis tool (in progress): final aim is to deliver pypi and conda packages (planned), port the documentation to readthedocs (planned).
- **Expand and rationalize diagnostics**, both from the scientific (e.g. uncertainty quantification), the technical (efficiency and code quality) and the visualization point of view. Looking forward to integrate diagnostics from other developers too!







### THANK YOU FOR YOUR ATTENTION!

The code is on GitHub and will be **Open Source** soon!

https://github.com/DestinE-Climate-DT/AQUA https://github.com/DestinE-Climate-DT/Climate-DT-catalog

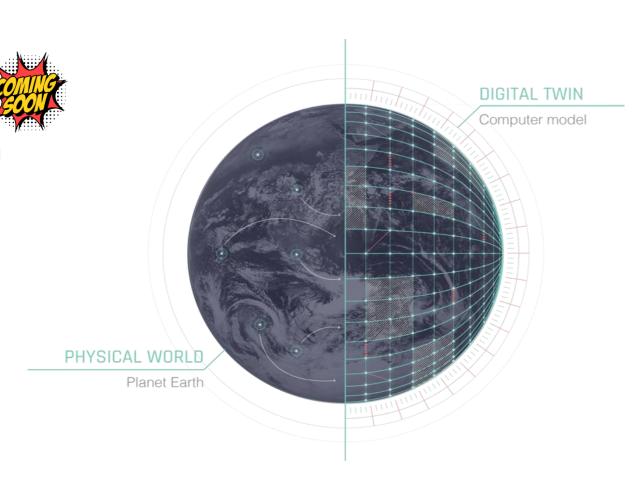




Fill out this form with your email and GitHub username to be added to the repo!

#### Aqua core team Contacts:

- m.nurisso@isac.cnr.it
- <u>silvia.caprioli@polito.it</u>
- jost.hardenberg@polito.it
- p.davini@isac.cnr.it
- natalia.nazarova@polito.it
- <u>supriyo.ghosh@bsc.es</u>





# **BACKUP SLIDES**

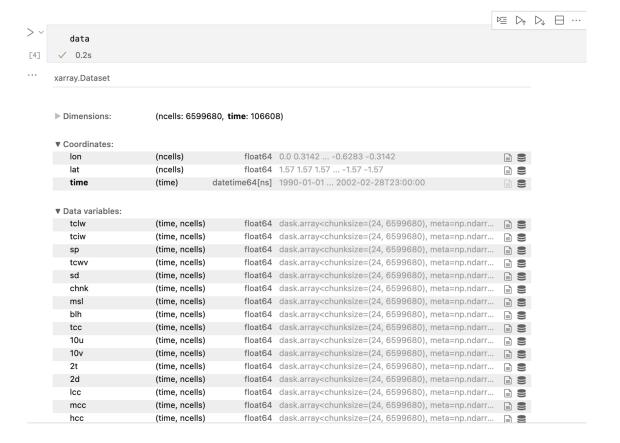
# **AQUA core concepts: the Reader**

Once a catalog is added the user can retrieve any dataset with two lines of code!



```
This is a lazy dask array!
```

```
from aqua import Reader
reader = Reader(model='IFS-NEMO', exp='historical-1990',
source='hourly-native-atm2d', regrid='r100')
data = reader.retrieve()
```





### Other available Reader methods

#### Time aggregation:

```
reader = Reader(model="IFS", exp="tco2559-ng5", source="ICMGG_atm2d")
data = reader.retrieve()
daily = reader.timmean(data, freq='daily')
```

#### **Spatial averaging:**

```
reader = Reader(model="IFS", exp="tco2559-ng5", source="ICMGG_atm2d")
data = reader.retrieve()
regional_mean = reader.fldmean(data, lon_limits=[-50, 50], lat_limits=[-10,20])
```

#### **Detrend:**

```
reader = Reader(model="IFS", exp="tco2559-ng5", source="ICMGG_atm2d")
data = reader.retrieve()
daily = reader.detrend(data['2t'], dim='time')
```

#### **Vertical interpolation**

```
reader = Reader(model="IFS", exp="tco2559-ng5", source="ICMU_atm3d",
regrid='r100')
data = reader.retrieve()
field = data['u'].isel(time=slice(0,5)).aqua.regrid()
interp = field.aqua.vertinterp(levels=[830, 835], units='hPa', method='linear')
```

### **Accessors:**

Please notice that all methods have accessors as data.aqua.fldmean() so that they can be called inline!



### THE LOW RESOLUTION ARCHIVE

LRA: AQUA had to address the extreme large volume of full resolution data in the Climate-DT Phase1. The solution was to create a tool which exploiting the parallelization capabilities of AQUA - based on dask - could postprocess high resolution data in few minutes moving from high spatial and temporal resolution to monthly 1deg x 1deg data

This is done combining AQUA fixer, regridding and time averaging functionalities and it is the foundation of AQUA monitoring.

On the long term we plan to deprecate the LRA if low resolution data will be produced on the model side.

In next release, LRA will be integrated in the command line so that it can be called with **`aqua Ira -c config.yaml`** 

```
#This include the option for the regridding
     target:
        resolution: r100
        frequency: monthly
       outdir: /pfs/lustrep3/projappl/project_465000454/data/AQUA/LRA
       tmpdir: /pfs/lustrep3/projappl/project_465000454/padavini/tmp
      loglevel: INFO
     # Set to True if lra-r100-monthly-zarr should be created and checked
     zarr: False
     verify_zarr: False
13
14
     slurm:
        partition: small
       username: padavini
       account: project 465000454
       time: 10:00:00
       mem: 256GB
20
21
      data:
22
       ICON:
23
         historical-1990:
24
           hourly-hpz10-atm2d:
25
             vars: ['mtpr', '2t', 'skt', 'msl', 'tcc', 'sd', 'tciw', 'tclw', 'msr', 'mslhf', 'msshf',
26
                 'msnswrf', 'msnlwrf', 'msdwlwrf', 'msdwswrf', 'mtnswrf', 'mtnlwrf', 'mtdwswrf']
27
             workers: 12
28
           hourly-hpz10-atm3d:
29
             vars: ['q', 't', 'u', 'v']
30
             workers: 6
31
           daily-hpz10-oce2d:
32
             workers: 16
33
             vars: ['avg_sithick', 'avg_siconc']
34
           daily-hpz10-oce3d:
35
             workers: 10
36
             vars: ['avg_thetao', 'avg_so']
```



# AQUA code and documentation

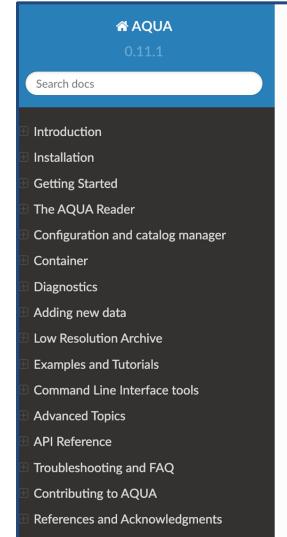
So far these are **two private repositories** on the Climate-DT **GitHub** (**AQUA**:

https://github.com/DestinE-Climate-DT/AQUA and
Climate-DT-catalog https://github.com/DestinEClimate-DT/Climate-DT-catalog)

**AQUA documentation** with **Sphinx** is available at <a href="https://aqua-web-climatedt.2.rahtiapp.fi/documentation/index.html">https://aqua-web-climatedt.2.rahtiapp.fi/documentation/index.html</a>

- General description
- How to install, how to run
- Illustrative examples
- API references
- FAQ for HPC deployment
- Container instructions

Frequent releases - current is v0.11.2



Welcome to AQUA's documentation!

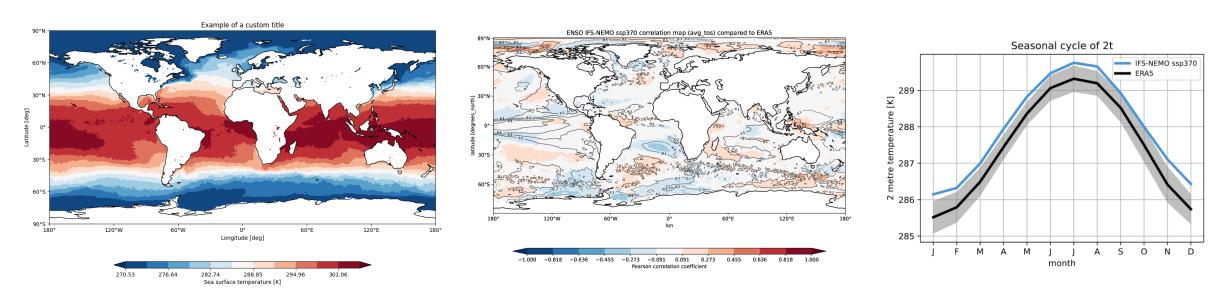
### Welcome to AQUA's documentation!

- Introduction
  - Overview of AQUA
  - Purpose
  - Key Features
  - Contributing
- Installation
  - Prerequisites
  - Installation with Mamba
  - Update of the environment
  - Installation on LUMI HPC
  - Installation on Levante HPC at DKRZ
  - Installation and use of the AQUA container
- Getting Started
  - Basic Concepts
  - Python installation
  - Catalog installation



# Graphical tools

Despite lagging a bit behind with respect to other features, some **basic functions for plotting** are already available within AQUA, as plot\_single\_map(), plot\_single\_map\_diff() and seasonal\_cycle()



These functions are used by the AQUA diagnostics but can be used on whatever xarray

