xcube

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GETTING STARTED

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xcube has been developed to generate, manipulate, analyse, and publish data cubes from EO data.

CHAPTER

OVERVIEW

xcube is an open-source Python package and toolkit that has been developed to provide Earth observation (EO) data in an analysis-ready form to users. xcube achieves this by carefully converting EO data sources into self-contained *data cubes* that can be published in the cloud.

1.1 Data Cube

The interpretation of the term *data cube* in the EO domain usually depends on the current context. It may refer to a data service such as Sentinel Hub, to some abstract API, or to a concrete set of spatial images that form a time-series.

This section briefly explains the specific concept of a data cube used in the xcube project - the xcube dataset.

1.2 xcube Dataset

1.2.1 Data Model

An xcube dataset contains one or more (geo-physical) data variables whose values are stored in cells of a common multidimensional, spatio-temporal grid. The dimensions are usually time, latitude, and longitude, however other dimensions may be present.

All xcube datasets are structured in the same way following a common data model. They are also self-describing by providing metadata for the cube and all cube's variables following the CF conventions. For details regarding the common data model, please refer to the *xcube Dataset Specification*.

A xcube dataset's in-memory representation in Python programs is an xarray.Dataset instance. Each dataset variable is represented by multi-dimensional xarray.DataArray that is arranged in non-overlapping, contiguous sub-regions called *data chunks*.

1.2.2 Data Chunks

Chunked variables allow for out-of-core computations of xcube dataset that don't fit in a single computer's RAM as data chunks can be processed independently from each other.

The way how dataset variables are sub-divided into smaller chunks - their *chunking* - has a substantial impact on processing performance and there is no single ideal chunking for all use cases. For time series analyses it is preferable to have chunks with a smaller spatial dimensions and larger time dimension, for spatial analyses and visualisation on using a map, the opposite is the case.

xcube provide tools for re-chunking of xcube datasets (*xcube chunk*, *xcube level*) and the xcube server (*xcube serve*) allows serving the same data cubes using different chunkings. For further reading have a look into the Chunking and Performance section of the xarray documentation.

1.2.3 Processing Model

When xcube datasets are opened, only the cube's structure and its metadata are loaded into memory. The actual data arrays of variables are loaded on-demand only, and only for chunks intersecting the desired sub-region.

Operations that generate new data variables from existing ones will be chunked in the same way. Therefore, such operation chains generate a processing graph providing a deferred, concurrent execution model.

1.2.4 Data Format

For the external, physical representation of xcube datasets we usually use the Zarr format. Zarr takes full advantage of data chunks and supports parallel processing of chunks that may originate from the local file system or from remote cloud storage such as S3 and GCS.

1.2.5 Python Packages

The xcube package builds heavily on Python's big data ecosystem for handling huge N-dimensional data arrays and exploiting cloud-based storage and processing resources. In particular, xcube's in-memory data model is provided by xarray, the memory management and processing model is provided through dask, and the external format is provided by zarr. xarray, dask, and zarr have increased their popularity for big data solutions over the last couple of years, for creating scalable and efficient EO data solutions.

1.3 Toolkit

On top of xarray, dask, zarr, and other popular Python data science packages, xcube provides various higher-level tools to generate, manipulate, and publish xcube datasets:

- CLI access, generate, modify, and analyse xcube datasets using the xcube tool;
- Python API access, generate, modify, and analyse xcube datasets via Python programs and notebooks;
- Web API and Server access, analyse, visualize xcube datasets via an xcube server;
- *Viewer App* publish and visualise xcube datasets using maps and time-series charts.

1.4 Workflows

The basic use case is to generate an xcube dataset and deploy it so that your users can access it:

- 1. generate an xcube dataset from some EO data sources using the xcube gen tool with a specific input processor.
- 2. optimize the generated xcube dataset with respect to specific use cases using the xcube chunk tool.
- 3. optimize the generated xcube dataset by consolidating metadata and elimination of empty chunks using *xcube optimize* and *xcube prune* tools.
- 4. deploy the optimized xcube dataset(s) to some location (e.g. on AWS S3) where users can access them.

Then you can:

- 5. access, analyse, modify, transform, visualise the data using the *Python API* and xarray API through Python programs or JupyterLab, or
- 6. extract data points by coordinates from a cube using the *xcube extract* tool, or
- 7. resample the cube in time to generate temporal aggregations using the *xcube resample* tool.

Another way to provide the data to users is via the *xcube server*, that provides a RESTful API and a WMTS. The latter is used to visualise spatial subsets of xcube datasets efficiently at any zoom level. To provide optimal visualisation and data extraction performance through the xcube server, xcube datasets may be prepared beforehand. Steps 8 to 10 are optional.

- 8. verify a dataset to be published conforms with the *xcube Dataset Specification* using the *xcube verify* tool.
- 9. adjust your dataset chunking to be optimal for generating spatial image tiles and generate a multi-resolution image pyramid using the *xcube chunk* and *xcube level* tools.
- 10. create a dataset variant optimal for time series-extraction again using the *xcube chunk* tool.
- 11. configure xcube datasets and publish them through the xcube server using the *xcube serve* tool.

You may then use a WMTS-compatible client to visualise the datasets or develop your own xcube server client that will make use of the xcube's REST API.

The easiest way to visualise your data is using the xcube *Viewer App*, a single-page web application that can be configured to work with xcube server URLs.

CHAPTER

TWO

EXAMPLES

When you follow the examples section you can build your first tiny xcube dataset and view it in the xcube-viewer by using the xcube server. The examples section is still growing and improving :)

Have fun exploring xcube!

Warning: This chapter is a work in progress and currently less than a draft.

2.1 Generating an xcube dataset

In the following example a tiny demo xcube dataset is generated.

2.1.1 Analysed Sea Surface Temperature over the Global Ocean

Input data for this example is located in the xcube repository. The input files contain analysed sea surface temperature and sea surface temperature anomaly over the global ocean and are provided by Copernicus Marine Environment Monitoring Service. The data is described in a dedicated Product User Manual.

Before starting the example, you need to activate the xcube environment:

```
$ conda activate xcube
```

If you want to take a look at the input data you can use cli/xcube dump to print out the metadata of a selected input file:

```
$ xcube dump examples/gen/data/20170605120000-UKMO-L4_GHRSST-SSTfnd-OSTIAanom-GLOB-v02.0-

$ fv02.0.nc
```

```
<xarray.Dataset>
Dimensions:
                  (lat: 720, lon: 1440, time: 1)
Coordinates:
  * lat
                  (lat) float32 -89.875 -89.625 -89.375 ... 89.375 89.625 89.875
  * lon
                  (lon) float32 0.125 0.375 0.625 ... 359.375 359.625 359.875
  * time
                  (time) object 2017-06-05 12:00:00
Data variables:
                  (time, lat, lon) float32 ...
   sst_anomaly
   analysed_sst (time, lat, lon) float32 ...
Attributes:
   Conventions:
                                CF-1.4
```

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title:	Global SST & Sea Ice Anomaly, L4 OSTIA, 0.25
summary:	A merged, multi-sensor L4 Foundation SST anom
references:	Donlon, C.J., Martin, M., Stark, J.D., Robert
institution:	UKMO
history:	Created from sst :temperature regridded with a
comment:	WARNING Some applications are unable to prope
license:	These data are available free of charge under
id:	UKMO-L4LRfnd_GLOB-OSTIAanom
naming_authority:	org.ghrsst
<pre>product_version:</pre>	2.0
uuid:	5c1665b7-06e8-499d-a281-857dcbfd07e2
gds_version_id:	2.0
<pre>netcdf_version_id:</pre>	3.6
date_created:	20170606T061737Z
<pre>start_time:</pre>	20170605 T000000Z
<pre>time_coverage_start:</pre>	20170605 T000000Z
<pre>stop_time:</pre>	20170606 T000000Z
time_coverage_end:	20170606 T000000Z
file_quality_level:	3
source:	UKMO-L4HRfnd-GLOB-OSTIA
platform:	Aqua, Envisat, NOAA-18, NOAA-19, MetOpA, MSG1
sensor:	AATSR, AMSR, AVHRR, AVHRR_GAC, SEVIRI, TMI
<pre>metadata_conventions:</pre>	Unidata Observation Dataset v1.0
<pre>metadata_link:</pre>	http://data.nodc.noaa.gov/NESDIS_DataCenters/
keywords:	Oceans > Ocean Temperature > Sea Surface Temp
keywords_vocabulary:	NASA Global Change Master Directory (GCMD) Sc
standard_name_vocabulary:	NetCDF Climate and Forecast (CF) Metadata Con
westernmost_longitude:	0.0
easternmost_longitude:	360.0
southernmost_latitude:	-90.0
northernmost_latitude:	90.0
spatial_resolution:	0.25 degree
<pre>geospatial_lat_units:</pre>	degrees_north
<pre>geospatial_lat_resolution:</pre>	0.25 degree
<pre>geospatial_lon_units:</pre>	degrees_east
<pre>geospatial_lon_resolution:</pre>	0.25 degree
acknowledgment:	Please acknowledge the use of these data with
creator_name:	Met Office as part of CMEMS
creator_email:	servicedesk.cmems@mercator-ocean.eu
creator_url:	http://marine.copernicus.eu/
project:	Group for High Resolution Sea Surface Tempera
publisher_name:	GHRSST Project Office
publisher_url:	http://www.ghrsst.org
publisher_email:	ghrsst-po@nceo.ac.uk
processing_level:	L4
cdm_data_type:	grid
uucu_cypei	<u></u>

Below an example xcube dataset will be created, which will contain the variable analysed_sst. The metadata for a specific variable can be viewed by:

\$ xcube dump examples/gen/data/20170605120000-UKMO-L4_GHRSST-SSTfnd-OSTIAanom-GLOB-v02.0-→ fv02.0.nc --var analysed_sst

```
<xarray.DataArray 'analysed_sst' (time: 1, lat: 720, lon: 1440)>
[1036800 values with dtype=float32]
Coordinates:
  * lat
             (lat) float32 -89.875 -89.625 -89.375 ... 89.375 89.625 89.875
  * lon
             (lon) float32 0.125 0.375 0.625 0.875 ... 359.375 359.625 359.875
 * time
             (time) object 2017-06-05 12:00:00
Attributes:
                    analysed sea surface temperature
    long_name:
    standard_name:
                    sea_surface_foundation_temperature
    type:
                    foundation
   units:
                    kelvin
   valid_min:
                    -300
   valid_max:
                    4500
    source:
                    UKMO-L4HRfnd-GLOB-OSTIA
    comment:
```

For creating a toy xcube dataset you can execute the command-line below. Please adjust the paths to your needs:

\$ xcube gen -o "your/output/path/demo_SST_xcube.zarr" -c examples/gen/config_files/xcube_ \$\infty\$ sst_demo_config.yml --sort examples/gen/data/*.nc

The configuration file specifies the input processor, which in this case is the default one. The output size is 10240, 5632. The bounding box of the data cube is given by output_region in the configuration file. The output format (output_writer_name) is defined as well. The chunking of the dimensions can be set by the chunksizes attribute of the output_writer_params parameter, and in the example configuration file the chunking is set for latitude and longitude. If the chunking is not set, a automatic chunking is applied. The spatial resampling method (output_resampling) is set to 'nearest' and the configuration file contains only one variable which will be included into the xcube dataset - 'analysed-sst'.

The Analysed Sea Surface Temperature data set contains the variable already as needed. This means no pixel masking needs to be applied. However, this might differ depending on the input data. You can take a look at a configuration file which takes Sentinel-3 Ocean and Land Colour Instrument (OLCI) as input files, which is a bit more complex. The advantage of using pixel expressions is, that the generated cube contains only valid pixels and the user of the data cube does not have to worry about something like land-masking or invalid values. Furthermore, the generated data cube is spatially regular. This means the data are aligned on a common spatial grid and cover the same region. The time stamps are kept from the input data set.

Caution: If you have input data that has file names not only varying with the time stamp but with e.g. A and B as well, you need to pass the input files in the desired order via a text file. Each line of the text file should contain the path to one input file. If you pass the input files in a desired order, then do not use the parameter **--sort** within the commandline interface.

2.1.2 Optimizing and pruning a xcube dataset

If you want to optimize your generated xcube dataset e.g. for publishing it in a xcube viewer via xcube serve you can use cli/xcube optimize:

\$ xcube optimize demo_SST_xcube.zarr -C

By executing the command above, an optimized xcube dataset called demo_SST_xcube-optimized.zarr will be created. You can take a look into the directory of the original xcube dataset and the optimized one, and you will notice that a file called .zmetadata. .zmetadata contains the information stored in .zattrs and .zarray of each variable of the xcube dataset and makes requests of metadata faster. The option -C optimizes coordinate variables by converting any chunked arrays into single, non-chunked, contiguous arrays.

For deleting empty chunks cli/xcube prune can be used. It deletes all data files associated with empty (NaN-only) chunks of an xcube dataset, and is restricted to the ZARR format.

\$ xcube prune demo_SST_xcube-optimized.zarr

The pruned xcube dataset is saved in place and does not need an output path. The size of the xcube dataset was 6,8 MB before pruning it and 6,5 MB afterwards. According to the output printed to the terminal, 30 block files were deleted.

The metadata of the xcube dataset can be viewed with cli/xcube dump as well:

\$ xcube dump demo_SST_xcube-optimized.zarr

```
<xarray.Dataset>
Dimensions:
                  (bnds: 2, lat: 5632, lon: 10240, time: 3)
Coordinates:
  * lat
                  (lat) float64 62.67 62.66 62.66 62.66 ... 48.01 48.0 48.0
    lat_bnds
                  (lat, bnds) float64 dask.array<shape=(5632, 2), chunksize=(5632, 2)>
                  (lon) float64 -16.0 -16.0 -15.99 -15.99 ... 10.66 10.66 10.67
  * lon
    lon_bnds
                  (lon, bnds) float64 dask.array<shape=(10240, 2), chunksize=(10240, 2)>
  *
   time
                  (time) datetime64[ns] 2017-06-05T12:00:00 ... 2017-06-07T12:00:00
                  (time, bnds) datetime64[ns] dask.array<shape=(3, 2), chunksize=(3, 2)>
    time_bnds
Dimensions without coordinates: bnds
Data variables:
    analysed_sst (time, lat, lon) float64 dask.array<shape=(3, 5632, 10240),
\rightarrow chunksize=(1, 704, 640)>
Attributes:
    acknowledgment:
                                Data Cube produced based on data provided by ...
   comment:
    contributor_name:
   contributor_role:
                                info@brockmann-consult.de
    creator_email:
                                Brockmann Consult GmbH
   creator_name:
                                https://www.brockmann-consult.de
   creator_url:
                                2019-09-25T08:50:32.169031
   date_modified:
   geospatial_lat_max:
                                62.666666666666666
   geospatial_lat_min:
                                48.0
   geospatial_lat_resolution:
                                0.002604166666666666
    geospatial_lat_units:
                                degrees_north
   geospatial_lon_max:
                                10.666666666666666
    geospatial_lon_min:
                                -16.0
   geospatial_lon_resolution: 0.002604166666666666666
   geospatial_lon_units:
                                degrees_east
   history:
                                xcube/reproj-snap-nc
   id:
                                demo-bc-sst-sns-l2c-v1
    institution:
                                Brockmann Consult GmbH
   keywords:
                                terms and conditions of the DCS4COP data dist...
   license:
   naming_authority:
                                bc
                                L2C
   processing_level:
   project:
                                xcube
                                info@brockmann-consult.de
   publisher_email:
   publisher_name:
                                Brockmann Consult GmbH
   publisher_url:
                                https://www.brockmann-consult.de
    references:
                                https://dcs4cop.eu/
```

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```
source:CMEMS Global SST & Sea Ice Anomaly Data Cubestandard_name_vocabulary:summary:2017-06-08T00:00:00.000000000time_coverage_end:2017-06-05T00:00:00.000000000time_icoverage_start:2017-06-05T00:00:00.000000000title:CMEMS Global SST Anomaly Data Cube
```

The metadata for the variable analysed_sst can be viewed:

\$ xcube dump demo_SST_xcube-optimized.zarr --var analysed_sst

```
<xarray.DataArray 'analysed_sst' (time: 3, lat: 5632, lon: 10240)>
dask.array<shape=(3, 5632, 10240), dtype=float64, chunksize=(1, 704, 640)>
Coordinates:
  * lat
             (lat) float64 62.67 62.66 62.66 62.66 ... 48.01 48.01 48.0 48.0
 * lon
             (lon) float64 -16.0 -16.0 -15.99 -15.99 ... 10.66 10.66 10.66 10.67
             (time) datetime64[ns] 2017-06-05T12:00:00 ... 2017-06-07T12:00:00
  * time
Attributes:
   comment:
   long_name:
                         analysed sea surface temperature
                         UKMO-L4HRfnd-GLOB-OSTIA
   source:
   spatial_resampling:
                         Nearest
                         sea_surface_foundation_temperature
   standard_name:
   type:
                         foundation
   units:
                         kelvin
   valid_max:
                         4500
   valid_min:
                         -300
```

Warning: This chapter is a work in progress and currently less than a draft.

2.2 Publishing xcube datasets

This example demonstrates how to run an xcube server to publish existing xcube datasets.

2.2.1 Running the server

To run the server on default port 8080 using the demo configuration:

\$ xcube serve --verbose -c examples/serve/demo/config.yml

To run the server using a particular xcube dataset path and styling information for a variable:

```
$ xcube serve --styles conc_chl=(0,20,"viridis") examples/serve/demo/cube-1-250-250.zarr
```

2.2.2 Test it

After starting the server, you can check the various functions provided by xcube Web API. To explore the functions, open

base-url>/openapi.html.

2.2.3 xcube Viewer

xcube datasets published through xcube serve can be visualised using the xcube-viewer web application. To do so, run xcube serve with the --open-viewer flag.

In order make this option usable, xcube-viewer must be installed and build:

- 1. Download and install yarn.
- 2. Download and build xcube-viewer:

```
$ git clone https://github.com/dcs4cop/xcube-viewer.git
$ cd xcube-viewer
$ yarn install
$ yarn build
```

3. Configure xcube serve so it finds the xcube-viewer On Linux (please adjust path):

```
$ export XCUBE_VIEWER_PATH=/abs/path/to/xcube-viewer/build
```

```
On Windows (please adjust path):
```

> SET XCUBE_VIEWER_PATH=/abs/path/to/xcube-viewer/build

4. Then run xcube serve --open-viewer:

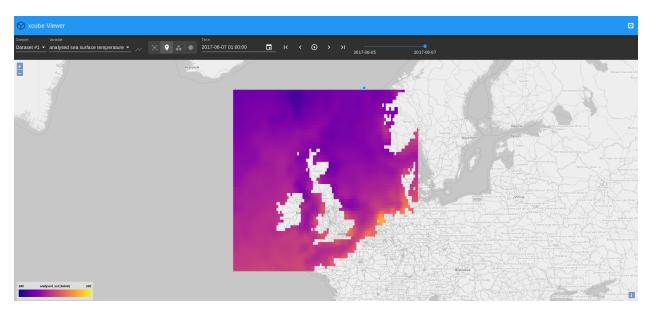
```
$ xcube serve --open-viewer --styles conc_chl=(0,20,"viridis") examples/serve/demo/cube-

$$ $$ -1-250-250.zarr
```

Viewing the generated xcube dataset described in the example Generating an xcube dataset:

```
$ xcube serve --open-viewer --styles "analysed_sst=(280,290,'plasma')" demo_SST_xcube-

→optimized.zarr
```



In case you get an error message "cannot reach server" on the very bottom of the web app's main window, refresh the page.

You can play around with the value range displayed in the viewer, here it is set to min=280K and max=290K. The colormap used for mapping can be modified as well and the colormaps provided by matplotlib can be used.

2.2.4 Other clients

There are example HTML pages for some tile server clients. They need to be run in a web server. If you don't have one, you can use Node's httpserver:

```
$ npm install -g httpserver
```

After starting both the xcube server and web server, e.g. on port 9090:

\$ httpserver -d -p 9090

you can run the client demos by following their links given below.

OpenLayers

- OpenLayers 4 Demo
- OpenLayers 4 Demo with WMTS

Cesium

To run the Cesium Demo first download Cesium and unpack the zip into the xcube serve source directory so that there exists an ./Cesium-x.y.z sub-directory. You may have to adapt the Cesium version number in the demo's HTML file.

CHAPTER

INSTALLATION

xcube can be installed from a released conda package, or directly from a copy of the source code repository.

The first two sections below give instructions for installation using conda, available as part of the miniconda distribution. If installation using conda proves to be unacceptably slow, mamba can be used instead (see *Installation using mamba*).

3.1 Installation from the conda package

Into a currently active, existing conda environment (>= Python 3.7)

\$ conda install -c conda-forge xcube

Into a new conda environment named xcube:

\$ conda create -c conda-forge -n xcube xcube

The argument to the -n option can be changed to create a differently named environment.

3.2 Installation from the source code repository

First, clone the repository and create a conda environment from it:

```
$ git clone https://github.com/dcs4cop/xcube.git
$ cd xcube
$ conda env create
```

From this point on, all instructions assume that your current directory is the root of the xcube repository.

The conda env create command above creates an environment according to the specifications in the environment. yml file in the repository, which by default takes the name xcube. Then, to activate the environment and install xcube from the repository:

```
$ conda activate xcube
$ pip install --no-deps --editable .
```

The second command installs xcube in 'editable mode', meaning that it will be run directly from the repository, and changes to the code in the repository will take immediate effect without reinstallation. (As an alternative to pip, the command python setup.py develop can be used, but this is no longer recommended. Among other things, pip has the advantage of allowing easy deinstallation of installed packages.)

To update the install to the latest repository version and update the environment to reflect to any changes in environment.yml:

```
$ conda activate xcube
$ git pull --force
$ conda env update -n xcube --file environment.yml --prune
```

To install pytest and run the unit test suite:

```
$ conda install pytest
$ pytest
```

To analyse test coverage (after installing pytest as above):

```
$ pytest --cov=xcube
```

To produce an HTML coverage report:

```
$ pytest --cov-report html --cov=xcube
```

3.3 Installation using mamba

Mamba is a dramatically faster drop-in replacement for the conda tool. Mamba itself can be installed using conda. If installation using conda proves to be unacceptably slow, it is recommended to install mamba, as follows:

```
$ conda create -n xcube python=3.8
$ conda activate xcube
$ conda install -c conda-forge mamba
```

This creates a conda environment called xcube, activates the environment, and installs mamba in it. To install xcube from its conda-forge package, you can now use:

```
$ mamba install -c conda-forge xcube
```

Alternatively, to install xcube directly from the repository:

```
$ git clone https://github.com/dcs4cop/xcube.git
$ cd xcube
$ mamba env create
$ pip install --no-deps --editable .
```

3.4 Docker

To start a demo using docker use the following commands

```
$ docker build -t [your name] .
$ docker run [your name]
```

\$ docker run -d -p [host port]:8080 [your name]

Example 1:

```
$ docker build -t xcube:0.10.0 .
$ docker run xcube:0.10.0
```

This will create the docker container and list the functionality of the xcube cli.

Example 2:

```
$ docker build -t xcube:0.10.0 .
$ docker run -d -p 8001:8080 xcube:0.10.0 "xcube serve -v --address 0.0.0.0 --port 8080_
--c /home/xcube/examples/serve/demo/config.yml"
$ docker ps
```

This will have started a service in the background which can be accessed through port 8001, as the startup of a service is configured as default behaviour.

CLI

The xcube command-line interface (CLI) is a single executable cli/xcube with several sub-commands comprising functions ranging from xcube dataset generation, over analysis and manipulation, to dataset publication.

4.1 Common Arguments and Options

Most of the commands operate on inputs that are xcube datasets. Such inputs are consistently named CUBE and provided as one or more command arguments. CUBE inputs may be a path into the local file system or a path into some object storage bucket, e.g. in AWS S3. Command inputs of other types are consistently called INPUT.

Many commands also output something, i.e. are writing files. The paths or names of such outputs are consistently provided by the -o OUTPUT or --output OUTPUT option. As the output is an option, there is usually a default value for it. If multiply file formats are supported, commands usually provide a -f FORMAT or --format FORMAT option. If omitted, the format may be guessed from the output's name.

4.2 Cube generation

4.2.1 xcube gen

Synopsis

Generate xcube dataset.

```
$ xcube gen --help
```

```
Usage: xcube gen [OPTIONS] [INPUT]...
Generate xcube dataset. Data cubes may be created in one go or successively
for all given inputs. Each input is expected to provide a single time slice
which may be appended, inserted or which may replace an existing time slice
in the output dataset. The input paths may be one or more input files or a
pattern that may contain wildcards '?', '*', and '**'. The input paths can
also be passed as lines of a text file. To do so, provide exactly one input
file with ".txt" extension which contains the actual input paths to be used.
Options:
    -P, --proc INPUT-PROCESSOR Input processor name. The available input
```

processor names and additional information

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	about input processors can be accessed by			
	calling xcube geninfo . Defaults to			
	"default", an input processor that can deal			
	with simple datasets whose variables have			
	dimensions ("lat", "lon") and conform with			
	the CF conventions.			
-c,config CONFIG	xcube dataset configuration file in YAML			
c, config confid	format. More than one config input file is			
	allowed. When passing several config files,			
	they are merged considering the order passed			
	via command line.			
o output OUTDUT	Output path. Defaults to 'out.zarr'			
-o,output OUTPUT				
-f,format FORMAT	Output format. Information about output			
	formats can be accessed by calling xcube gen			
	info. If omitted, the format will be			
_	guessed from the given output path.			
-S,size SIZE	Output size in pixels using format			
	" <width>,<height>".</height></width>			
-R,region REGION	Output region using format " <lon-min>,<lat-< td=""></lat-<></lon-min>			
	<pre>min>,<lon-max>,<lat-max>"</lat-max></lon-max></pre>			
variables,vars VARIABLES	Variables to be included in output. Comma-			
	separated list of names which may contain			
	wildcard characters "*" and "?".			
resampling				
→ [Average Bilinear Cubic CubicSp	line Lanczos Max Median Min Mode Nearest Q1 Q3]			
	Fallback spatial resampling algorithm to be			
	used for all variables. Defaults to			
	'Nearest'. The choices for the resampling			
	algorithm are: ['Average', 'Bilinear',			
	'Cubic', 'CubicSpline', 'Lanczos', 'Max',			
	'Median', 'Min', 'Mode', 'Nearest', 'Q1',			
	'Q3']			
-a,append	Deprecated. The command will now always			
a, append	create, insert, replace, or append input			
	slices.			
nnof				
prof	Collect profiling information and dump			
	results after processing.			
no_sort	The input file list will not be sorted			
	before creating the xcube dataset. If			
	no_sort parameter is passed, the order of			
	the input list will be kept. This parameter			
	should be used for better performance,			
	provided that the input file list is in			
	correct order (continuous time).			
-I,info	Displays additional information about format			
	options or about input processors.			
dry_run	Just read and process inputs, but don't			
	produce any outputs.			
help	Show this message and exit.			

Below is the ouput of a xcube gen --info call showing five input processors installed via plugins.

\$ xcube gen --info

```
input processors to be used with option --proc:
  default
                                    Single-scene NetCDF/CF inputs in xcube standard
\rightarrow format
  rbins-seviri-highroc-scene-12
                                    RBINS SEVIRI HIGHROC single-scene Level-2 NetCDF
⊣inputs
  rbins-seviri-highroc-daily-12
                                    RBINS SEVIRI HIGHROC daily Level-2 NetCDF inputs
                                    SNAP Sentinel-3 OLCI HIGHROC Level-2 NetCDF inputs
  snap-olci-highroc-l2
                                    SNAP Sentinel-3 OLCI CyanoAlert Level-2 NetCDF inputs
  snap-olci-cyanoalert-l2
  vito-s2plus-12
                                    VITO Sentinel-2 Plus Level 2 NetCDF inputs
For more input processors use existing "xcube-gen-..." plugins from the github_
→organisation DCS4COP or write own plugin.
Output formats to be used with option --format:
                          (*.zarr)
                                        Zarr file format (http://zarr.readthedocs.io)
  zarr
 netcdf4
                          (*.nc)
                                        NetCDF-4 file format
                          (*.csv)
                                        CSV file format
  CSV
                                        In-memory dataset I/O
  mem
                          (*.mem)
```

Configuration File

Configuration files passed to xcube gen via the -c, --config option use YAML format. Multiple configuration files may be given. In this case all configurations are merged into a single one. Parameter values will be overwritten by subsequent configurations if they are scalars. If they are objects / mappings, their values will be deeply merged.

The following parameters can be used in the configuration files:

input_processor [str] The name of an input processor. See -P, --proc option above.

- **Default** The default value is 'default', xcube's default input processor. It can ingest and process inputs that
 - use an EPSG: 4326 (or compatible) grid;
 - have 1-D lon and lat coordinate variables using WGS84 coordinates and decimal degrees;
 - have a decodable 1-D time coordinate or define the one of the following global attribute pairs time_coverage_start and time_coverage_end, time_start and time_end or time_stop;
 - provide data variables with the dimensions time, lat, lon, in this order.
 - conform to the **`CF Conventions`_**.
- **output_size** [[int, int]] The spatial dimension sizes of the output dataset given as number of grid cells in longitude and latitude direction (width and height).
- **output_region** [[float, float, float]] The spatial extent of output datasets given as a bounding box [lat-min, lat-min, lon-max, lat-max] using decimal degrees.
- **output_variables** [[*variable-definitions*]] The definition of variables that will be included in the output dataset. Each variable definition may be just a name or a mapping from a name to variable attributes. If it is just a name it must be the name of an existing variable either in the INPUT or in processed_variables. If the variable

definition is a mapping, some of the attributes affect the way how variables are processed. All but the name attributes become variable metadata in the output.

name [str] The new name of the variable in the output.

valid_pixel_expression [str] An expression used to mask this variable, see *Expressions*. The expression identifies all valid pixels in each INPUT.

resampling [str] The resampling method used. See --resampling option above.

Default By default, all variables in INPUT will occur in output.

processed_variables [[variable-definitions]] The definition of variables that will be produced or processed after reading each INPUT. The main purpose is to generate intermediate variables that can be referred to in the expression in other variable definitions in processed_variables and valid_pixel_expression in variable definitions in output_variables. The following attributes are recognised:

expression [str] An expression used to produce this variable, see *Expressions*.

output_writer_name [str] The name of a supported output format. May be one of 'zarr', 'netcdf4', 'mem'.

Default 'zarr'

output_writer_params [str] A mapping that defines parameters that are passed to output writer denoted by **output_writer_name**. Through the **output_writer_params** a packing of the variables may be defined. If not specified the default does not apply any packing which results in:

```
_FillValue: nan
dtype: dtype('float32')
```

and for coordinate variables

dtype: dtype('int64')

The user may specify a different packing variables, which might be useful for reducing the storage size of the datacubes. Currently it is only implemented for zarr format. This may be done by passing the parameters for packing as the following:

```
output_writer_params:
    packing:
    analysed_sst:
        scale_factor: 0.07324442274239326
        add_offset: -300.0
        dtype: 'uint16'
        _FillValue: 0.65535
```

Furthermore the compressor may be defined as well by, if not specified the default compressor (cname='lz4', clevel=5, shuffle=SHUFFLE, blocksize=0) is used.

```
output_writer_params:
    compressor:
        cname: 'zstd'
        clevel: 1
        shuffle: 2
```

output_metadata [[*attribute-definitions*]] General metadata that will be present in the output dataset as global attributes. You can put any common CF attributes here.

Any attributes that are mappings will be "flattened" by concatenating the attribute names using the underscrore character. For example,:

```
publisher:
  name: "Brockmann Consult GmbH"
  url: "https://www.brockmann-consult.de"
```

will create the two entries:

publisher_name: "Brockmann Consult GmbH"
publisher_url: "https://www.brockmann-consult.de"

Expressions

Expressions are plain text values of the expression and valid_pixel_expression attributes of the variable definitions in the processed_variables and output_variables parameters. The expression syntax is that of standard Python. xcube gen uses expressions to produce new variables listed in processed_variables and to mask variables by the valid_pixel_expression.

An expression may refer any variables in the INPUT datasets and any variables defined by the processed_variables parameter. Expressions may make use of most of the standard Python operators and may apply all numpy ufuncs to referred variables. Also most of the xarray.DataArray API may be used on variables within an expression.

In order to utilise flagged variables, the syntax variable_name.flag_name can be used in expressions. According to the CF Conventions, flagged variables are variables whose metadata include the attributes flag_meanings and flag_values and/or flag_masks. The flag_meanings attribute enumerates the allowed values for flag_name. The flag attributes must be present in the variables of each INPUT.

Example

An example that uses a configuration file only:

```
$ xcube gen --config ./config.yml /data/eo-data/SST/2018/**/*.nc
```

An example that uses the default input processor and passes all other configuration via command-line options:

Some input processors have been developed for specific EO data sources used within the DCS4COP project. They may serve as examples how to develop input processor plug-ins:

- xcube-gen-rbins
- xcube-gen-bc
- xcube-gen-vito

Python API

The related Python API function is xcube.core.gen.gen_cube().

4.2.2 xcube grid

Attention: This tool will likely change in the near future.

Synopsis

Find spatial xcube dataset resolutions and adjust bounding boxes.

```
$ xcube grid --help
```

```
Usage: xcube grid [OPTIONS] COMMAND [ARGS]...
  Find spatial xcube dataset resolutions and adjust bounding boxes.
  We find suitable resolutions with respect to a possibly regional fixed
  Earth grid and adjust regional spatial bounding boxes to that grid. We
  also try to select the resolutions such that they are taken from a certain
  level of a multi-resolution pyramid whose level resolutions increase by a
  factor of two.
  The graticule at a given resolution level L within the grid is given by
      RES(L) = COVERAGE * HEIGHT(L)
      \text{HEIGHT}(L) = \text{HEIGHT}_0 * 2 \wedge L
      LON(L, I) = LON_MIN + I * HEIGHT_0 * RES(L)
      LAT(L, J) = LAT_MIN + J * HEIGHT_0 * RES(L)
  With
                Grid resolution in degrees.
      RES:
                Number of vertical grid cells for given level
      HEIGHT:
      HEIGHT_0: Number of vertical grid cells at lowest resolution level.
  Let WIDTH and HEIGHT be the number of horizontal and vertical grid cells
  of a global grid at a certain LEVEL with WIDTH * RES = 360 and HEIGHT *
  RES = 180, then we also force HEIGHT = TILE * 2 ^ LEVEL.
Options:
  --help Show this message and exit.
Commands:
  abox
          Adjust a bounding box to a fixed Earth grid.
  levels List levels for a resolution or a tile size.
          List resolutions close to a target resolution.
  res
```

Example: Find suitable target resolution for a \sim 300m (Sentinel 3 OLCI FR resolution) fixed Earth grid within a deviation of 5%.

\$ xcube grid res 300m -D 5%										
TILE	LEVEL	HEIGHT	INV_RES	RES (deg)	RES (m)	, DELTA_	_RES (%)			
540	7	69120	384	0.0026041666	666666665	289.9	-3.4			
4140	4	66240	368	0.0027173913	04347826	302.5	0.8			
8100	3	64800	360	0.0027777777	77777778	309.2	3.1			

289.9m is close enough and provides 7 resolution levels, which is good. Its inverse resolution is 384, which is the fixed Earth grid identifier.

We want to see if the resolution pyramid also supports a resolution close to 10m (Sentinel 2 MSI resolution).

```
$ xcube grid levels 384 -m 6
```

```
LEVEL
       HEIGHT
               INV_RES RES (deg)
                                      RES (m)
                       0.333333333333333333333
       540
               3
                                              37106.5
0
       1080
1
               6
                       0.16666666666666666
                                              18553.2
2
       2160
               12
                       0.08333333333333333333
                                              9276.6
. . .
11
       1105920 6144
                       12
       2211840 12288
                       8.138020833333333e-05
                                              9.1
13
       4423680 24576
                       4.0690104166666664e-05 4.5
```

This indicates we have a resolution of 9.1m at level 12.

Lets assume we have xcube dataset region with longitude from 0 to 5 degrees and latitudes from 50 to 52.5 degrees. What is the adjusted bounding box on a fixed Earth grid with the inverse resolution 384?

\$ xcube grid abox 0,50,5,52.5 384

```
Orig. box coord. = 0.0, 50.0, 5.0, 52.5
Adj. box coord. = 0.0,49.21875,5.625,53.4375
Orig. box WKT
                 = POLYGON ((0.0 50.0, 5.0 50.0, 5.0 52.5, 0.0 52.5, 0.0 50.0))
                 = POLYGON ((0.0 49.21875, 5.625 49.21875, 5.625 53.4375, 0.0 53.4375, 0.
Adj. box WKT
→0 49.21875))
Grid size = 2160 x 1620 cells
with
  TILE
            = 540
           = 7
 LEVEL
  INV_RES
           = 384
  RES (deg) = 0.0026041666666666665
  RES (m)
            = 289.89450727414993
```

Note, to check bounding box WKTs, you can use the handy Wicket tool.

4.3 Cube computation

4.3.1 xcube compute

Synopsis

Compute a cube variable from other cube variables using a user-provided Python function.

```
$ xcube compute --help
```

```
Usage: xcube compute [OPTIONS] SCRIPT [CUBE]...
  Compute a cube from one or more other cubes.
  The command computes a cube variable from other cube variables in CUBEs
  using a user-provided Python function in SCRIPT.
  The SCRIPT must define a function named "compute":
      def compute(*input_vars: numpy.ndarray,
                  input_params: Mapping[str, Any] = None,
                  dim_coords: Mapping[str, np.ndarray] = None,
                  dim_ranges: Mapping[str, Tuple[int, int]] = None) \
                  -> numpy.ndarray:
          # Compute new numpy array from inputs
          # output_array = ...
          return output_array
  where input_vars are numpy arrays (chunks) in the order given by VARIABLES
  or given by the variable names returned by an optional "initialize" function
  that my be defined in SCRIPT too, see below. input_params is a mapping of
  parameter names to values according to PARAMS or the ones returned by the
  aforesaid "initialize" function. dim_coords is a mapping from dimension name
  to coordinate labels for the current chunk to be computed. dim_ranges is a
  mapping from dimension name to index ranges into coordinate arrays of the
  cube.
  The SCRIPT may define a function named "initialize":
      def initialize(input_cubes: Sequence[xr.Dataset],
                     input_var_names: Sequence[str],
                     input_params: Mapping[str, Any]) \
                     -> Tuple[Sequence[str], Mapping[str, Any]]:
          # Compute new variable names and/or new parameters
          # new_input_var_names = ...
          # new_input_params = ...
          return new_input_var_names, new_input_params
  where input_cubes are the respective CUBEs, input_var_names the respective
  VARIABLES, and input_params are the respective PARAMS. The "initialize"
  function can be used to validate the data cubes, extract the desired
  variables in desired order and to provide some extra processing parameters
```

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```
passed to the "compute" function.
  Note that if no input variable names are specified, no variables are passed
  to the "compute" function.
  The SCRIPT may also define a function named "finalize":
      def finalize(output_cube: xr.Dataset,
                   input_params: Mapping[str, Any]) \
                   -> Optional[xr.Dataset]:
          # Optionally modify output_cube and return it or return None
          return output_cube
  If defined, the "finalize" function will be called before the command writes
  the new cube and then exists. The functions may perform a cleaning up or
  perform side effects such as write the cube to some sink. If the functions
  returns None, the CLI will *not* write any cube data.
Options:
  --variables, --vars VARIABLES Comma-separated list of variable names.
                                 Parameters passed as 'input_params' dict to
  -p, --params PARAMS
                                 compute() and init() functions in SCRIPT.
  -o, --output OUTPUT
                                 Output path. Defaults to 'out.zarr'
  -f, --format FORMAT
                                 Output format.
  -N, --name NAME
                                 Output variable's name.
  -D, --dtype DTYPE
                                 Output variable's data type.
  --help
                                 Show this message and exit.
```

Example

\$ xcube compute s3-olci-cube.zarr ./algoithms/s3-olci-ndvi.py

with ./algoithms/s3-olci-ndvi.py being:

TODO

Python API

The related Python API function is xcube.core.compute.compute_cube().

4.4 Cube inspection

4.4.1 xcube dump

Synopsis

Dump contents of a dataset.

```
$ xcube dump --help
```

```
Usage: xcube dump [OPTIONS] INPUT

Dump contents of an input dataset.

Options:

--variable, --var VARIABLE Name of a variable (multiple allowed).

-E, --encoding Dump also variable encoding information.

--help Show this message and exit.
```

Example

```
$ xcube dump xcube_cube.zarr
```

4.4.2 xcube verify

Synopsis

Perform cube verification.

```
$ xcube verify --help
```

```
Usage: xcube verify [OPTIONS] CUBE
Perform cube verification.
The tool verifies that CUBE
* defines the dimensions "time", "lat", "lon";
* has corresponding "time", "lat", "lon" coordinate variables and that they
are valid, e.g. 1-D, non-empty, using correct units;
* has valid bounds variables for "time", "lat", "lon" coordinate
variables, if any;
* has any data variables and that they are valid, e.g. min. 3-D, all have
same dimensions, have at least dimensions "time", "lat", "lon".
* spatial coordinates and their corresponding bounds (if exist) are equidistant
```

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```
and monotonically increasing or decreasing.
If INPUT is a valid xcube dataset, the tool returns exit code 0. Otherwise a
violation report is written to stdout and the tool returns exit code 3.
Options:
    --help Show this message and exit.
```

Python API

The related Python API functions are

- xcube.core.verify.verify_cube(), and
- xcube.core.verify.assert_cube().

4.5 Cube data extraction

4.5.1 xcube extract

Synopsis

Extract cube points.

```
$ xcube extract --help
```

```
Usage: xcube extract [OPTIONS] CUBE POINTS
  Extract cube points.
  Extracts data cells from CUBE at coordinates given in each POINTS record and
  writes the resulting values to given output path and format.
  POINTS must be a CSV file that provides at least the columns "lon", "lat",
  and "time". The "lon" and "lat" columns provide a point's location in
  decimal degrees. The "time" column provides a point's date or date-time. Its
  format should preferably be ISO, but other formats may work as well.
Options:
  -o, --output OUTPUT Output path. If omitted, output is written to stdout.
  -f, --format FORMAT Output format. Currently, only 'csv' is supported.
 -C, --coords
                       Include cube cell coordinates in output.
  -B, --bounds
                       Include cube cell coordinate boundaries (if any) in
                       output.
  -I, --indexes
                       Include cube cell indexes in output.
                       Include point values as reference in output.
  -R, --refs
  --help
                       Show this message and exit.
```

Example

\$ xcube extract xcube_cube.zarr -o point_data.csv -Cb --indexes --refs

Python API

Related Python API functions are

- xcube.core.extract.get_cube_values_for_points(),
- xcube.core.extract.get_cube_point_indexes(), and
- xcube.core.extract.get_cube_values_for_indexes().

4.6 Cube manipulation

4.6.1 xcube chunk

Synopsis

(Re-)chunk xcube dataset.

\$ xcube chunk --help

```
Usage: xcube chunk [OPTIONS] CUBE
  (Re-)chunk xcube dataset. Changes the external chunking of all variables of
  CUBE according to CHUNKS and writes the result to OUTPUT.
  Note: There is a possibly more efficient way to (re-)chunk datasets through
  the dedicated tool "rechunker", see https://rechunker.readthedocs.io.
Options:
  -o, --output OUTPUT Output path. Defaults to 'out.zarr'
  -f, --format FORMAT
                      Format of the output. If not given, guessed from
                       OUTPUT.
  -p, --params PARAMS Parameters specific for the output format. Comma-
                       separated list of <key>=<value> pairs.
  -C, --chunks CHUNKS Chunk sizes for each dimension. Comma-separated list of
                       <dim>=<size> pairs, e.g. "time=1,lat=270,lon=270"
  -q, --quiet
                       Disable output of log messages to the console entirely.
                       Note, this will also suppress error and warning
                       messages.
  -v, --verbose
                       Enable output of log messages to the console. Has no
                       effect if --quiet/-q is used. May be given multiple
                       times to control the level of log messages, i.e., -v
                       refers to level INFO, -vv to DETAIL, -vvv to DEBUG,
                       -vvvv to TRACE. If omitted, the log level of the
                       console is WARNING.
  --help
                       Show this message and exit.
```

Example

Python API

The related Python API function is xcube.core.chunk.chunk_dataset().

4.6.2 xcube edit

Please note, the xcube edit command has been deprecated since xcube 0.13. It will be removed in later versions of xcube. Please use xcube patch instead.

Synopsis

Edit metadata of an xcube dataset.

\$ xcube edit --help

```
Usage: xcube edit [OPTIONS] CUBE
  Edit the metadata of an xcube dataset. Edits the metadata of a given CUBE.
  The command currently works only for data cubes using ZARR format.
Options:
  -o, --output OUTPUT
                           Output path. The placeholder "{input}" will be
                           replaced by the input's filename without extension
                           (such as ".zarr"). Defaults to
                           "{input}-edited.zarr".
  -M, --metadata METADATA The metadata of the cube is edited. The metadata to
                           be changed should be passed over in a single yml
                           file.
  -C, --coords
                           Update the metadata of the coordinates of the xcube
                           dataset.
  -I, --in-place
                           Edit the cube in place. Ignores output path.
  --help
                           Show this message and exit.
```

Examples

The global attributes of the demo xcube dataset demo cube-1-250-250.zarr in the examples folder do not contain the creators name not an url. Furthermore the long name of the variable 'conc_chl' is 'Chlorophylll concentration', with too many l's. This can be fixed by using xcube edit. A yml-file defining the key words to be changed with the new content has to be created. The demo yml is saved in the examples folder.

Edit the metadata of the existing xcube dataset cube-1-250-250-edited.zarr:

```
$ xcube edit /examples/serve/demo/cube-1-250-250.zarr -M examples/edit/edit_metadata_

$\operatorname{cube-1-250-250.yml -0 cube-1-250-250-edited.zarr}$
```

The global attributes below, which are related to the xcube dataset coodrinates cannot be manually edited.

- geospatial_lon_min
- geospatial_lon_max
- geospatial_lon_units
- geospatial_lon_resolution
- geospatial_lat_min
- geospatial_lat_max
- geospatial_lat_units
- geospatial_lat_resolution
- time_coverage_start
- time_coverage_end

If you wish to update these attributes, you can use the commandline parameter -C:

\$ xcube edit /examples/serve/demo/cube-1-250-250.zarr -C -o cube-1-250-250-edited.zarr

The -C will update the coordinate attributes based on information derived directly from the cube.

Python API

The related Python API function is xcube.core.edit.edit_metadata().

4.6.3 xcube level

Synopsis

Generate multi-resolution levels.

```
$ xcube level --help
```

```
Usage: xcube level [OPTIONS] INPUT
  Generate multi-resolution levels.
  Transform the given dataset by INPUT into the levels of a multi-level
  pyramid with spatial resolution decreasing by a factor of two in both
  spatial dimensions and write the result to directory OUTPUT.
  INPUT may be an S3 object storage URL of the form "s3://<bucket>/<path>" or
  "https://<endpoint>".
Options:
                                  Output path. If omitted, "INPUT.levels" will
  -o, --output OUTPUT
                                  be used. You can also use S3 object storage
                                  URLs of the form "s3://<bucket>/<path>" or
                                  "https://<endpoint>"
                                  Link the INPUT instead of converting it to a
  -L, --link
                                  level zero dataset. Use with care, as the
```

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	INPUT's internal spatial chunk sizes may be
	inappropriate for imaging purposes.
-t,tile-size TILE_SIZE	Tile size, given as single integer number or
	<pre>as <tile-width>,<tile-height>. If omitted,</tile-height></tile-width></pre>
	the tile size will be derived from the
	INPUT's internal spatial chunk sizes. If the
	INPUT is not chunked, tile size will be 512.
-n,num-levels-max NUM_LEVELS	S_MAX
	Maximum number of levels to generate. If not
	given, the number of levels will be derived
	from spatial dimension and tile sizes.
-A,agg-methods AGG_METHODS	Aggregation method(s) to be used for data
	variables. Either one of "first", "min",
	"max", "mean", "median", "auto" or list of
	assignments to individual variables using
	the notation
	<pre>"<var1>=<method1>,<var2>=<method2>,"</method2></var2></method1></var1></pre>
	Defaults to "first".
-r,replace	Whether to replace an existing dataset at
	OUTPUT .
-a,anon	For S3 inputs or outputs, whether the access
	is anonymous. By default, credentials are
	required.
-q,quiet	Disable output of log messages to the
	console entirely. Note, this will also
	suppress error and warning messages.
-v,verbose	Enable output of log messages to the
	console. Has no effect ifquiet/-q is
	used. May be given multiple times to control
	the level of log messages, i.e., -v refers
	to level INFO, -vv to DETAIL, -vvv to DEBUG,
	-vvvv to TRACE. If omitted, the log level of
	the console is WARNING.
help	Show this message and exit.
L	

Example

\$ xcube level --link -t 720 data/cubes/test-cube.zarr

Python API

The related Python API functions are

- xcube.core.level.compute_levels(),
- xcube.core.level.read_levels(), and
- xcube.core.level.write_levels().

4.6.4 xcube optimize

Synopsis

Optimize xcube dataset for faster access.

```
$ xcube optimize --help
Usage: xcube optimize [OPTIONS] CUBE
  Optimize xcube dataset for faster access.
  Reduces the number of metadata and coordinate data files in xcube dataset
  given by CUBE. Consolidated cubes open much faster especially from remote
  locations, e.g. in object storage, because obviously much less HTTP requests
  are required to fetch initial cube meta information. That is, it merges all
  metadata files into a single top-level JSON file ".zmetadata". Optionally,
  it removes any chunking of coordinate variables so they comprise a single
  binary data file instead of one file per data chunk. The primary usage of
  this command is to optimize data cubes for cloud object storage. The command
  currently works only for data cubes using ZARR format.
Options:
  -o, --output OUTPUT Output path. The placeholder "<built-in function
                       input>" will be replaced by the input's filename
                       without extension (such as ".zarr"). Defaults to
                       "{input}-optimized.zarr".
                       Optimize cube in place. Ignores output path.
  -I, --in-place
  -C, --coords
                       Also optimize coordinate variables by converting any
                       chunked arrays into single, non-chunked, contiguous
                       arrays.
```

Examples

--help

Write an cube with consolidated metadata to cube-optimized.zarr:

\$ xcube optimize ./cube.zarr

Write an optimized cube with consolidated metadata and consolidated coordinate variables to optimized/cube.zarr (directory optimized must exist):

```
$ xcube optimize -C -o ./optimized/cube.zarr ./cube.zarr
```

Optimize a cube in-place with consolidated metadata and consolidated coordinate variables:

Show this message and exit.

```
$ xcube optimize -IC ./cube.zarr
```

Python API

The related Python API function is xcube.core.optimize.optimize_dataset().

4.6.5 xcube patch

Synopsis

Patch and consolidate the metadata of a xcube dataset.

```
$ xcube patch --help
```

Usage: xcube patch [OPTIONS] DATASET		
Patch and consolidate the metadata of a dataset.		
DATASET can be either a local filesystem path or a URL. It must point to either a Zarr dataset (*.zarr) or a xcube multi-level dataset (*.levels). Additional storage options for a given protocol may be passed by the OPTIONS option.		
In METADATA, the spe	cial attribute value "delete" can be used to remove	
that attribute from dataset or array metadata.		
Options:		
-	The metadata to be patched. Must be a JSON or YAML file using Zarr consolidated metadata format.	
options OPTIONS	Protocol-specific storage options (see fsspec). Must be a JSON or YAML file.	
-q,quiet	Disable output of log messages to the console entirely. Note, this will also suppress error and warning messages.	
-v,verbose	Enable output of log messages to the console. Has no effect ifquiet/-q is used. May be given multiple times to control the level of log messages, i.e., -v refers to level INFO, -vv to DETAIL, -vvv to DEBUG, -vvvv to TRACE. If omitted, the log level of the console is WARNING.	
-d,dry-run	Do not change any data, just report what would have been changed.	
help	Show this message and exit.	

Patch file example

Patch files use the Zarr Consolidated Metadata Format, v1. For example, the following patch file (YAML) will delete the global attribute TileSize and change the value of the attribute long_name of variable conc_chl:

```
zarr_consolidated_format: 1
metadata:
   .zattrs:
    TileSize: __delete__
   conc_chl/.zattrs:
    long_name: Chlorophyll concentration
```

Storage options file example

Here is a storage options file for the "s3" protocol that provides credentials for AWS S3 access:

```
key: AJDKJCLSKKA
secret: kjkl456lkj45632k45j631
```

Usage example

\$ xcube patch s3://my-cubes-bucket/test.zarr --metadata patch.yml -v

4.6.6 xcube prune

Delete empty chunks.

Attention: This tool will likely be integrated into xcube optimize in the near future.

\$ xcube prune --help

```
Usage: xcube prune [OPTIONS] DATASET
  Delete empty chunks. Deletes all data files associated with empty (NaN-only)
  chunks in given DATASET, which must have Zarr format.
Options:
                Disable output of log messages to the console entirely. Note,
  -q, --quiet
                 this will also suppress error and warning messages.
  -v, --verbose Enable output of log messages to the console. Has no effect
                 if --quiet/-q is used. May be given multiple times to control
                 the level of log messages, i.e., -v refers to level INFO, -vv
                 to DETAIL, -vvv to DEBUG, -vvvv to TRACE. If omitted, the log
                 level of the console is WARNING.
  --dry-run
                 Just read and process input, but don't produce any output.
  --help
                 Show this message and exit.
```

A related Python API function is xcube.core.optimize.get_empty_dataset_chunks().

4.6.7 xcube resample

Synopsis

Resample data along the time dimension.

\$ xcube resample --help Usage: xcube resample [OPTIONS] CUBE Resample data along the time dimension. Options: -c, --config CONFIG xcube dataset configuration file in YAML format. More than one config input file is allowed When passing several config files, they are merged considering the order passed via command line. -o, --output OUTPUT Output path. Defaults to 'out.zarr'. -f, --format [zarr|netcdf4|mem] Output format. If omitted, format will be quessed **from output** path. Comma-separated list of names of variables --variables, --vars VARIABLES to be included. -M, --method TEXT Temporal resampling method. Available downsampling methods are 'count', 'first', 'last', 'min', 'max', 'sum', 'prod', 'mean', 'median', 'std', 'var', the upsampling methods are 'asfreq', 'ffill', 'bfill', 'pad', 'nearest', 'interpolate'. If the upsampling method **is** 'interpolate', the option '--kind' will be used, if given. Other upsampling methods that select existing values honour the '--tolerance' option. Defaults to 'mean'. -F, --frequency TEXT Temporal aggregation frequency. Use format "<count><offset>" where <offset> is one of 'H', 'D', 'W', 'M', 'Q', 'Y'. Use 'all' to aggregate all time steps included in the dataset.Defaults to '1D'. -0, --offset TEXT Offset used to adjust the resampled time labels. Uses same syntax as frequency. Some Pandas date offset strings are supported as well. -B, --base INTEGER For frequencies that evenly subdivide 1 day, the origin of the aggregated intervals. For example, **for** '24H' frequency, base could range **from** 0 through 23. Defaults to 0. -K, --kind TEXT Interpolation kind which will be used if upsampling method is 'interpolation'. May be

(continued from previous page)

	<pre>one of 'zero', 'slinear', 'quadratic',</pre>
	<pre>'cubic', 'linear', 'nearest', 'previous',</pre>
	<pre>'next' where 'zero', 'slinear', 'quadratic',</pre>
	<pre>'cubic' refer to a spline interpolation of</pre>
	zeroth, first, second or third order;
	'previous' and 'next' simply return the
	previous or next value of the point. For
	more info refer to
	<pre>scipy.interpolate.interp1d(). Defaults to</pre>
	'linear'.
-T,tolerance TEXT	Tolerance for selective upsampling methods.
	Uses same syntax as frequency. If the time
	delta exceeds the tolerance, fill values
	(NaN) will be used. Defaults to the given
	frequency.
-q,quiet	Disable output of log messages to the
	console entirely. Note, this will also
	suppress error and warning messages.
-v,verbose	Enable output of log messages to the
	console. Has no effect if quiet/-q is
	used. May be given multiple times to control
	the level of log messages, i.e., -v refers
	to level INFO, -vv to DETAIL, -vvv to DEBUG,
	-vvvv to TRACE. If omitted, the log level of
	the console is WARNING.
dry-run	Just read and process inputs, but don't
-	produce any outputs.
help	Show this message and exit.

Examples

Upsampling example:

```
$ xcube resample --vars conc_chl,conc_tsm -F 12H -T 6H -M interpolation -K linear_

→examples/serve/demo/cube.nc
```

Downsampling example:

```
$ xcube resample --vars conc_chl,conc_tsm -F 3D -M mean -M std -M count examples/serve/

→demo/cube.nc
```

Python API

The related Python API function is xcube.core.resample.resample_in_time().

4.6.8 xcube vars2dim

Synopsis

Convert cube variables into new dimension.

```
$ xcube vars2dim --help
Usage: xcube vars2dim [OPTIONS] CUBE
  Convert cube variables into new dimension. Moves all variables of CUBE
  into a single new variable <var-name> with a new dimension DIM-NAME and
  writes the results to OUTPUT.
Options:
  --variable, --var VARIABLE Name of the new variable that includes all
                              variables. Defaults to "data".
  -D, --dim_name DIM-NAME
                              Name of the new dimension into variables.
                              Defaults to "var".
  -o, --output OUTPUT
                              Output path. If omitted, 'INPUT-vars2dim.FORMAT'
                              will be used.
  -f, --format FORMAT
                              Format of the output. If not given, guessed from
                              OUTPUT.
  --help
                              Show this message and exit.
```

Python API

The related Python API function is xcube.core.vars2dim.vars_to_dim().

4.7 Cube conversion

4.8 Cube publication

4.8.1 xcube serve

Synopsis

Serve data cubes via web service.

xcube serve starts a light-weight web server that provides various services based on xcube datasets:

- Catalogue services to query for xcube datasets and their variables and dimensions, and feature collections;
- Tile map service, with some OGC WMTS 1.0 compatibility (REST and KVP APIs);
- Dataset services to extract subsets like time-series and profiles for e.g. JavaScript clients.

\$ xcube serve --help

Usage: xcube serve [OPTIONS] [PATHS...] Run the xcube Server for the given configuration and/or the given raster dataset paths given by PATHS. Each of the PATHS arguments can point to a raster dataset such as a Zarr directory (*.zarr), an xcube multi-level Zarr dataset (*.levels), a NetCDF file (*.nc), or a GeoTIFF/COG file (*.tiff). If one of PATHS is a directory that is not a dataset itself, it is scanned **for** readable raster datasets. The --show ASSET option can be used to inspect the current configuration of the server. ASSET is one of: apis outputs the list of APIs provided by the server endpoints outputs the list of all endpoints provided by the server openapi outputs the OpenAPI document representing this server config outputs the effective server configuration configschema outputs the JSON Schema for the server configuration The ASSET may be suffixed by ".yaml" or ".json" forcing the respective output format. The default format is YAML. Note, if --show is provided, the ASSET will be shown and the program will exit immediately. Options: --framework FRAMEWORK Web server framework. Defaults to "tornado" -p, --port PORT Service port number. Defaults to 8080 Service address. Defaults to "0.0.0.0". -a, --address ADDRESS -c, --config CONFIG Configuration YAML or JSON file. If multiple configuration files are passed, they will be →merged **in** order. --base-dir BASE_DIR Directory used to resolve relative paths in CONFIG files. Defaults to the parent directory of (last) CONFIG file. --prefix URL_PREFIX Prefix path to be used **for** all endpoint URLs. May include template variables, e.g., "api/{version}". Prefix path to be used for reverse endpoint --revprefix REVERSE_URL_PREFIX URLs that may be reported by server responses. May include template variables, e.g., "/proxy/{port}". Defaults to value of URL_PREFIX. --traceperf Whether to output extra performance logs. --update-after TIME Check **for** server configuration updates every TIME seconds. --stop-after TIME Unconditionally stop service after TIME seconds. --show ASSET Show ASSET and exit. Possible values for ASSET are 'apis', 'endpoints', 'openapi'

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	<pre>'config', 'configschema' optionally suffixed</pre>
	by '.yaml' or '.json'.
open-viewer	After starting the server, open xcube Viewer
	in a browser tab.
-q,quiet	Disable output of log messages to the
	console entirely. Note, this will also
	suppress error and warning messages.
-v,verbose	Enable output of log messages to the
	console. Has no effect if quiet/-q is
	used. May be given multiple times to control
	the level of log messages, i.e., -v refers
	to level INFO, -vv to DETAIL, -vvv to DEBUG,
	-vvvv to TRACE. If omitted, the log level of
	the console is WARNING.
help	Show this message and exit.

Configuration File

The xcube server is used to configure the xcube datasets to be published.

xcube datasets are any datasets that

- that comply to Unidata's CDM and to the CF Conventions;
- that can be opened with the xarray Python library;
- that have variables that have the dimensions and shape (lat, lon) or (time, lat, lon);
- that have 1D-coordinate variables corresponding to the dimensions;
- that have their spatial grid defined in arbitrary spatial coordinate reference systems.

The xcube server supports xcube datasets stored as local NetCDF files, as well as Zarr directories in the local file system or remote object storage. Remote Zarr datasets must be stored AWS S3 compatible object storage.

As an example, here is the configuration of the demo server. The parts of the demo configuration file are explained in detail further down.

Some hints before, which are not addressed in the server demo configuration file. To increase imaging performance, xcube datasets can be converted to multi-resolution pyramids using the *xcube level* tool. In the configuration, the format must be set to 'levels'. Leveled xcube datasets are configured this way:

```
Datasets:
```

```
    Identifier: my_multi_level_dataset
Title: My Multi-Level Dataset
FileSystem: file
Path: my_multi_level_dataset.levels
    ...
```

To increase time-series extraction performance, xcube datasets may be rechunked with larger chunk size in the time dimension using the *xcube chunk* tool. In the xcube server configuration a hidden dataset is given, and the it is referred to by the non-hidden, actual dataset using the TimeSeriesDataset setting:

Datasets:

```
Identifier: my_dataset
Title: My Dataset
FileSystem: file
Path: my_dataset.zarr
TimeSeriesDataset: my_dataset_opt_for_ts
Identifier: my_dataset_opt_for_ts
Title: My Dataset optimized for Time-Series
FileSystem: file
Path: my_ts_opt_dataset.zarr
Hidden: True
```

Server Demo Configuration File

The server configuration file consists of various parts, some of them are necessary others are optional. Here the demo configuration file used in the *example* is explained in detail.

The configuration file consists of five main parts authentication, dataset attribution, datasets, place groups and styles.

Authentication [optional]

In order to display data via xcube-viewer exclusively to registered and authorized users, the data served by xcube serve may be protected by adding Authentication to the server configuration. In order to ensure protection, an *Authority* and an *Audience* needs to be provided. Here authentication by Auth0 is used. Please note the trailing slash in the "Authority" URL.

```
Authentication:
Authority: https://xcube-dev.eu.auth0.com/
Audience: https://xcube-dev/api/
```

Example of OIDC configuration for Keycloak. Please note that there is no trailing slash in the "Authority" URL.

```
Authentication:
Authority: https://kc.brockmann-consult.de/auth/realms/AVL
Audience: avl-xc-api
```

Dataset Attribution [optional]

Dataset Attribution may be added to the server via *DatasetAttribution*.

```
DatasetAttribution:
    - "© by Brockmann Consult GmbH 2020, contains modified Copernicus Data 2019, processed...
    - by ESA"
    - "© by EU H2020 CyanoAlert project"
```

Base Directory [optional]

A typical xcube server configuration comprises many paths, and relative paths of known configuration parameters are resolved against the base_dir configuration parameter.

base_dir: s3://<bucket>/<path-to-your>/<resources>/

However, for values of parameters passed to user functions that represent paths in user code, this cannot be done automatically. For such situations, expressions can be used. An expression is any string between "\${"` and `"}" in a configuration value. An expression can contain the variables base_dir (a string), ctx the current server context (type xcube.webapi.datasets.DatasetsContext), as well as the function resolve_config_path(path) that is used to make a path absolut with respect to base_dir and to normalize it. For example

```
Augmentation:
Path: augmentation/metadata.py
Function: metadata:update_metadata
InputParameters:
    bands_config: ${resolve_config_path("../common/bands.yaml")}
```

Viewer Configuration [optional]

The xcube server endpoint /viewer/config/{*path} allows for configuring the viewer accessible via endpoint / viewer. The actual source for the configuration items is configured by xcube server configuration using the new entry Viewer/Configuration/Path, for example:

```
Viewer:
Configuration:
Path: s3://<bucket>/<viewer-config-dir-path>
```

Path [mandatory] must be an absolute filesystem path or a S3 path as in the example above. It points to a directory that is expected to contain the the viewer configuration file *config.json* among other configuration resources, such as custom favicon.ico or logo.png. The file config.json should conform to the [configuration JSON Schema](https://github.com/dcs4cop/xcube-viewer/blob/master/src/resources/config.schema.json). All its values are optional, if not provided, [default values](https://github.com/dcs4cop/xcube-viewer/blob/master/src/resources/config.json) are used instead.

Datasets [mandatory]

In order to publish selected xcube datasets via xcube serve, the datasets need to be described in the server configuration.

Remotely stored xcube Datasets

The following configuration snippet demonstrates how to publish static (persistent) xcube datasets stored in S3compatible object storage:

```
Datasets:
    - Identifier: remote
    Title: Remote OLCI L2C cube for region SNS
    BoundingBox: [0.0, 50, 5.0, 52.5]
```

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```
FileSystem: s3
Endpoint: "https://s3.eu-central-1.amazonaws.com"
Path: xcube-examples/OLCI-SNS-RAW-CUBE-2.zarr
Region: eu-central-1
Anonymous: true
Style: default
ChunkCacheSize: 250M
PlaceGroups:
    - PlaceGroupRef: inside-cube
    - PlaceGroupRef: outside-cube
AccessControl:
    RequiredScopes:
        - read:datasets
```

The above example of how to specify a xcube dataset to be served above is using a datacube stored in an S3 bucket within the Amazon Cloud. Please have a closer look at the parameter *Anonymous: true*. This means, the datasets permissions are set to public read in your source s3 bucket. If you have a dataset that is not public-read, set *Anonymous: false*. Furthermore, you need to have valid credentials on the machine where the server runs. Credentials may be saved either in a file called .aws/credentials with content like below:

[default] aws_access_key_id=AKIAIOSFODNN7EXAMPLE aws_secret_access_key=wJalrXUtnFEMI/K7MDENG/bPxRfiCYEXAMPLEKEY

Or they may be exported as environment variables AWS_SECRET_ACCESS_KEY and AWS_ACCESS_KEY_ID.

Further down an example for a *locally stored xcube datasets* will be given, as well as an example of *dynamic xcube datasets*.

Identifier [mandatory] is a unique ID for each xcube dataset, it is ment for machine-to-machine interaction and therefore does not have to be a fancy human-readable name.

Title [optional] should be understandable for humans. This title that will be displayed within the viewer for the dataset selection. If omitted, the key title from the dataset metadata will be used. If that is missing too, the identifier will be used.

BoundingBox [optional] may be set in order to restrict the region which is served from a certain datacube. The notation of the *BoundingBox* is [lon_min,lat_min,lon_max,lat_max].

FileSystem [mandatory] is set to "s3" which lets xcube serve know, that the datacube is located in the cloud.

Endpoint [mandatory] contains information about the cloud provider endpoint, this will differ if you use a different cloud provider.

Path [mandatory] leads to the specific location of the datacube. The particular datacube is stored in an OpenTelecom-Cloud S3 bucket called "xcube-examples" and the datacube is called "OLCI-SNS-RAW-CUBE-2.zarr".

Region [optional] is the region where the specified cloud provider is operating.

Styles [optional] influence the visualization of the xucbe dataset in the xcube viewer if specified in the server configuration file. The usage of *Styles* is described in section *styles*.

PlaceGroups [optional] allow to associate places (e.g. polygons or point-location) with a particular xcube dataset. Several different place groups may be connected to a xcube dataset, these different place groups are distinguished by the *PlaceGroupRef.* The configuration of *PlaceGroups* is described in section *place groups*.

AccessControl [optional] can only be used when providing *authentication*. Datasets may be protected by configuring the *RequiredScopes* entry whose value is a list of required scopes, e.g. "read:datasets".

Locally stored xcube Datasets

The following configuration snippet demonstrates how to publish static (persistent) xcube datasets stored in the local filesystem:

```
- Identifier: local
 Title: Local OLCI L2C cube for region SNS
 BoundingBox: [0.0, 50, 5.0, 52.5]
 FileSystem: file
 Path: cube-1-250-250.zarr
 Style: default
 TimeSeriesDataset: local_ts
 Augmentation:
   Path: compute_extra_vars.py
   Function: compute_variables
   InputParameters:
      factor_chl: 0.2
      factor_tsm: 0.7
 PlaceGroups:
    - PlaceGroupRef: inside-cube
    - PlaceGroupRef: outside-cube
 AccessControl:
   IsSubstitute: true
```

Most of the configuration of locally stored datasets is equal to the configuration of remotely stored xcube datasets.

FileSystem [mandatory] is set to "file" which lets xcube serve know, that the datacube is locally stored.

TimeSeriesDataset [optional] is not bound to local datasets, this parameter may be used for remotely stored datasets as well. By using this parameter a time optimized datacube will be used for generating the time series. The configuration of this time optimized datacube is shown below. By adding *Hidden* with *true* to the dataset configuration, the time optimized datacube will not appear among the displayed datasets in xcube viewer.

```
# Will not appear at all, because it is a "hidden" resource
- Identifier: local_ts
Title: 'local' optimized for time-series
BoundingBox: [0.0, 50, 5.0, 52.5]
FileSystem: file
Path: cube-5-100-200.zarr
Hidden: true
Style: default
```

Augmentation [optional] augments data cubes by new variables computed on-the-fly, the generation of the on-the-fly variables depends on the implementation of the python module specified in the *Path* within the *Augmentation* configuration.

AccessControl [optional] can only be used when providing *authentication*. By passing the *IsSubstitute* flag a dataset disappears for authorized requests. This might be useful for showing a demo dataset in the viewer for user who are not logged in.

Dynamic xcube Datasets

There is the possibility to define dynamic xcube datasets that are computed on-the-fly. Given here is an example that obtains daily or weekly averages of an xcube dataset named "local".

```
- Identifier: local_1w
 Title: OLCI weekly L3 cube for region SNS computed from local L2C cube
 BoundingBox: [0.0, 50, 5.0, 52.5]
 FileSystem: memory
 Path: resample_in_time.py
 Function: compute_dataset
 InputDatasets: ["local"]
 InputParameters:
   period: 1W
   incl_stdev: True
 Style: default
 PlaceGroups:
   - PlaceGroupRef: inside-cube
   - PlaceGroupRef: outside-cube
 AccessControl:
   IsSubstitute: True
```

FileSystem [mandatory] must be "memory" for dynamically generated datasets.

Path [mandatory] points to a Python module. Can be a Python file, a package, or a Zip file.

Function [mandatory, mutually exclusive with *Class*] references a function in the Python file given by *Path*. Must be suffixed by colon-separated module name, if *Path* references a package or Zip file. The function receives one or more datasets of type xarray.Dataset as defined by *InputDatasets* and optional keyword-arguments as given by *InputParameters*, if any. It must return a new xarray.Dataset with same spatial coordinates as the inputs. If "resample_in_time.py" is compressed among any other modules in a zip archive, the original module name must be indicated by the prefix to the function name:

```
Path: modules.zip
Function: resample_in_time:compute_dataset
InputDatasets: ["local"]
```

Class [mandatory, mutually exclusive with *Function*] references a callable in the Python file given by *Path*. Must be suffixed by colon-separated module name, if *Path* references a package or Zip file. The callable is either a class derived from xcube.core.mldataset.MultiLevelDataset or a function that returns an instance of xcube.core.mldataset.MultiLevelDataset. The callable receives one or more datasets of type xcube.core.mldataset.MultiLevelDataset as defined by *InputDatasets* and optional keyword-arguments as given by *InputParameters*, if any.

InputDatasets [mandatory] specifies the input datasets passed to Function or Class.

InputParameters [mandatory] specifies optional keyword arguments passed to *Function* or *Class*. In the example, *InputParameters* defines which kind of resampling should be performed.

Again, the dataset may be associated with place groups.

Place Groups [optional]

Place groups are specified in a similar manner compared to specifying datasets within a server. Place groups may be stored e.g. in shapefiles or a geoJson.

```
PlaceGroups:
- Identifier: outside-cube
Title: Points outside the cube
Path: places/outside-cube.geojson
PropertyMapping:
    image: ${resolve_config_path("images/outside-cube/${ID}.jpg")}
```

Identifier [mandatory] is a unique ID for each place group, it is the one xcube serve uses to associate a place group to a particular dataset.

Title [mandatory] should be understandable for humans and this is the title that will be displayed within the viewer for the place selection if the selected xcube dataset contains a place group.

Path [mandatory] defines where the file storing the place group is located. Please note that the paths within the example config are relative.

PropertyMapping [mandatory] determines which information contained within the place group should be used for selecting a certain location of the given place group. This depends very strongly of the data used. In the above example, the image URL is determined by a feature's ID property.

Property Mappings

The entry *PropertyMapping* is used to map a set of well-known properties (or roles) to the actual properties provided by a place feature in a place group. For example, the well-known properties are used to in xcube viewer to display information about the currently selected place. The possible well-known properties are:

- label: The property that provides a label for the place, if any. Defaults to to case-insensitive names label, title, name, id in xcube viewer.
- color: The property that provides a place's color. Defaults to the case-insensitive name color in xcube viewer.
- image: The property that provides a place's image URL, if any. Defaults to case-insensitive names image, img, picture, pic in xcube viewer.
- description: The property that provides a place's description text, if any. Defaults to case-insensitive names description, desc, abstract, comment in xcube viewer.

In the following example, a place's label is provided by the place feature's NAME property, while an image is provided by the place feature's IMG_URL property:

```
PlaceGroups:
    Identifier: my_group
    ...
    PropertyMapping:
        label: NAME
        image: IMG_URL
```

The values on the right side may either **be** feature property names or **contain** them as placeholders in the form \${PROPERTY}.

Styles [optional]

Within the *Styles* section, colorbars may be defined which should be used initially for a certain variable of a dataset, as well as the value ranges. For xcube viewer version 0.3.0 or higher the colorbars and the value ranges may be adjusted by the user within the xcube viewer.

```
Styles:
  - Identifier: default
    ColorMappings:
      conc_chl:
        ColorBar: plasma
        ValueRange: [0., 24.]
      conc_tsm:
        ColorBar: PuBuGn
        ValueRange: [0., 100.]
      kd489:
        ColorBar: jet
        ValueRange: [0., 6.]
      rgb:
        Red:
          Variable: conc_chl
          ValueRange: [0., 24.]
        Green:
          Variable: conc_tsm
          ValueRange: [0., 100.]
        Blue:
          Variable: kd489
          ValueRange: [0., 6.]
```

The *ColorMapping* may be specified for each variable of the datasets to be served. If not specified, xcube server will try to extract default values from attributes of dataset variables. The default value ranges are determined by:

- xcube-specific variable attributes color_value_min and color_value_max;
- The CF variable attributes valid_min, valid_max or valid_range.
- Or otherwise, the value range [0, 1] is assumed.

The colorbar name can be set using the

- xcube-specific variable attribute color_bar_name;
- Otherwise, the default colorbar name will be viridis.

The special name *rgb* may be used to generate an RGB-image from any other three dataset variables used for the individual *Red*, *Green* and *Blue* channels of the resulting image. An example is shown in the configuration above.

Colormaps may be reversed by using name suffix "_r". They also can have alpha blending indicated by name suffix "_alpha". Both, reversed and alpha blending is possible as well and can be configured by name suffix "_r_alpha".

```
Styles:
    - Identifier: default
    ColorMappings:
        conc_chl:
        ColorBar: plasma_r_alpha
        ValueRange: [0., 24.]
```

Example

```
xcube serve --port 8080 --config ./examples/serve/demo/config.yml --verbose
```

Server Demo Configuration File for DataStores

The server configuration file consists of various parts, some of them are necessary, others are optional. Here the demo stores configuration file used in the *example stores* is explained in detail.

This configuration file differs only in one part compared to section *Server Demo Configuration File: data stores*. The other main parts (*authentication, dataset attribution, place groups*, and *styles*) can be used in combination with *data stores*.

DataStores [mandatory]

Datasets, which are stored in the same location, may be configured in the configuration file using DataStores.

```
DataStores:
- Identifier: edc
StoreId: s3
StoreParams:
    root: xcube-dcfs/edc-xc-viewer-data
    max_depth: 1
    storage_options:
        anon: true
        # client_kwargs:
        # endpoint_url: https://s3.eu-central-1.amazonaws.com
Datasets:
        - Path: "*2.zarr"
        Style: default
        # ChunkCacheSize: 1G
```

Identifier [mandatory] is a unique ID for each DataStore.

StoreID [mandatory] can be file for locally stored datasets and s3 for datasets located in the cloud.

StoreParams [mandatory]

root [mandatory] states a common beginning part of the paths of the served datasets.

max_depth [optional] if wildcard is used in *Dataset Path* this indicated how far the server should step down and serve the discovered datasets.

storage_options [optional] is necessary when serving datasets from the cloud. With *anon* the accessibility is configured, if the datasets are public-read, *anon* is set to "true", "false" indicates they are protected. Credentials may be set by keywords *key* and *secret*.

Datasets [optional] if not specified, every dataset in the indicated location supported by xcube will be read and served by xcube serve. In order to filter certain datasets you can list Paths that shall be served by xcube serve. *Path* may contain wildcards. Each Dataset entry may have *Styles* and *PlaceGroups* associated with them, the same way as described in section *Server Demo Configuration File*.

Example Stores

xcube serve --port 8080 --config ./examples/serve/demo/config-with-stores.yml --verbose

xcube Server: WMTS, catalogue, data access, tile, feature, time-series services for_ →xarray-enabled data cubes, version [I 190924 17:08:54 service:228] configuration file 'D:\\Projects\\xcube\\examples\\serve\ →\demo\\config.yml' successfully loaded [I 190924 17:08:54 service:158] service running, listening on localhost:8080, try http:// →localhost:8080/datasets [I 190924 17:08:54 service:159] press CTRL+C to stop service

Example Azure Blob Storage filesystem Stores

xcube server includes support for Azure Blob Storage filesystem by a data store *abfs*. This enables access to data cubes (*.zarr* or *.levels*) in Azure blob storage as shown here:

```
DataStores:
- Identifier: siec
StoreId: abfs
StoreParams:
    root: my_blob_container
    max_depth: 1
    storage_options:
    anon: true
    account_name: "xxx"
    account_key': "xxx"
    # or
    # connection_string: "xxx"
Datasets:
    - Path: "*.levels"
    Style: default
```

Web API

The xcube server has a dedicated self describing Web API Documentation. After starting the server, you can check the various functions provided by xcube Web API. To explore the functions, open

hase-url>/openapi.html.

The xcube server implements the OGC WMTS RESTful and KVP architectural styles of the OGC WMTS 1.0.0 specification. The following operations are supported:

- GetCapabilities: /xcube/wmts/1.0.0/WMTSCapabilities.xml
- GetTile: /xcube/wmts/1.0.0/tile/{DatasetName}/{VarName}/{TileMatrix}/{TileCol}/ {TileRow}.png
- GetFeatureInfo: in progress

CHAPTER

FIVE

PYTHON API

5.1 Cube I/O

5.2 Cube generation

xcube.core.new.new_cube(title='Test Cube', width=360, height=180, x_name='lon', y_name='lat',

x_dtype='float64', y_dtype=None, x_units='degrees_east', y_units='degrees_north', x_res=1.0, y_res=None, x_start=- 180.0, y_start=- 90.0, inverse_y=False, time_name='time', time_dtype='datetime64[s]', time_units='seconds since 1970-01-01T00:00:00', time_calendar='proleptic_gregorian', time_periods=5, time_freq='D', time_start='2010-01-01T00:00:00', use_cftime=False, drop_bounds=False, variables=None, crs=None, crs_name=None)

Create a new empty cube. Useful for creating cubes templates with predefined coordinate variables and metadata. The function is also heavily used by xcube's unit tests.

The values of the *variables* dictionary can be either constants, array-like objects, or functions that compute their return value from passed coordinate indexes. The expected signature is::

def my_func(time: int, y: int, x: int) -> Union[bool, int, float]

Parameters

- title (str) A title. Defaults to 'Test Cube'.
- width (int) Horizontal number of grid cells. Defaults to 360.
- height (int) Vertical number of grid cells. Defaults to 180.
- **x_name** (str) Name of the x coordinate variable. Defaults to 'lon'.
- y_name (str) Name of the y coordinate variable. Defaults to 'lat'.
- **x_dtype** (str) Data type of x coordinates. Defaults to 'float64'.
- **y_dtype** Data type of y coordinates. Defaults to 'float64'.
- **x_units** (str) Units of the x coordinates. Defaults to 'degrees_east'.
- y_units (str) Units of the y coordinates. Defaults to 'degrees_north'.
- **x_start** (float) Minimum x value. Defaults to -180.
- **y_start** (float) Minimum y value. Defaults to -90.
- **x_res** (float) Spatial resolution in x-direction. Defaults to 1.0.
- y_res Spatial resolution in y-direction. Defaults to 1.0.

- **inverse_y** (bool) Whether to create an inverse y axis. Defaults to False.
- time_name (str) Name of the time coordinate variable. Defaults to 'time'.
- time_periods (int) Number of time steps. Defaults to 5.
- time_freq (str) Duration of each time step. Defaults to `1D'.
- time_start (str) First time value. Defaults to '2010-01-01T00:00:00'.
- **time_dtype** (str) Numpy data type for time coordinates. Defaults to 'datetime64[s]'. If used, parameter 'use_cftime' must be False.
- time_units (str) Units for time coordinates. Defaults to 'seconds since 1970-01-01T00:00:00'.
- time_calendar (str) Calender for time coordinates. Defaults to 'proleptic_gregorian'.
- **use_cftime** (bool) If True, the time will be given as data types according to the 'cftime' package. If used, the time_calendar parameter must be also be given with an appropriate value such as 'gregorian' or 'julian'. If used, parameter 'time_dtype' must be None.
- **drop_bounds** (bool) If True, coordinate bounds variables are not created. Defaults to False.
- variables Dictionary of data variables to be added. None by default.
- crs pyproj-compatible CRS string or instance of pyproj.CRS or None
- crs_name Name of the variable that will hold the CRS information. Ignored, if crs is not given.

Returns A cube instance

5.3 Cube computation

5.4 Cube data extraction

5.5 Cube manipulation

Unchunk dataset variables in-place.

Parameters

- **dataset_path** (str) Path to ZARR dataset directory.
- var_names Optional list of variable names.
- coords_only (bool) Un-chunk coordinate variables only.

xcube.core.optimize_dataset(input_path: str, output_path: Optional[str] = None, in_place: bool = False, unchunk_coords: Union[bool, str, Sequence[str]] = False, exception type: Type[Exception] = <class 'ValueError'>)

Optimize a dataset for faster access.

Reduces the number of metadata and coordinate data files in xcube dataset given by given by *dataset_path*. Consolidated cubes open much faster from remote locations, e.g. in object storage, because obviously much less

HTTP requests are required to fetch initial cube meta information. That is, it merges all metadata files into a single top-level JSON file ".zmetadata".

If *unchunk_coords* is given, it also removes any chunking of coordinate variables so they comprise a single binary data file instead of one file per data chunk. The primary usage of this function is to optimize data cubes for cloud object storage. The function currently works only for data cubes using Zarr format. *unchunk_coords* can be a name, or list of names of the coordinate variable(s) to be consolidated. If boolean True is used, coordinate all variables will be consolidated.

Parameters

- **input_path** (str) Path to input dataset with ZARR format.
- **output_path** (str) Path to output dataset with ZARR format. May contain "{input}" template string, which is replaced by the input path's file name without file name extension.
- **in_place** (bool) Whether to modify the dataset in place. If False, a copy is made and *output_path* must be given.
- **unchunk_coords** The name of a coordinate variable or a list of coordinate variables whose chunks should be consolidated. Pass **True** to consolidate chunks of all coordinate variables.
- **exception_type** Type of exception to be used on value errors.

5.6 Cube subsetting

5.7 Cube masking

class xcube.core.maskset.MaskSet(flag_var: xarray.DataArray)

A set of mask variables derived from a variable *flag_var* with the following CF attributes:

- One or both of *flag_masks* and *flag_values*
- flag_meanings (always required)

See https://cfconventions.org/Data/cf-conventions/cf-conventions-1.9/cf-conventions.html#flags for details on the use of these attributes.

Each mask is represented by an *xarray.DataArray*, has the name of the flag, is of type *numpy.unit8*, and has the dimensions of the given *flag_var*.

Parameters flag_var – an *xarray.DataArray* that defines flag values. The CF attributes *flag_meanings* and one or both of *flag_masks* and *flag_values* are expected to exist and be valid.

classmethod get_mask_sets(*dataset: xarray.Dataset*) \rightarrow Dict[str, *xcube.core.maskset.MaskSet*] For each "flag" variable in given *dataset*, turn it into a MaskSet, store it in a dictionary.

Parameters dataset – The dataset

Returns A mapping of flag names to MaskSet. Will be empty if there

are no flag variables in dataset.

5.8 Rasterisation of Features

5.9 Cube metadata

- 5.10 Cube verification
- 5.11 Multi-resolution pyramids

5.12 Utilities

5.13 Plugin Development

has_extension(*point: str, name: str*) \rightarrow bool Test if an extension with given *point* and *name* is registered.

Return type bool

Parameters

- **point** (str) extension point identifier
- **name** (str) extension name

Returns True, if extension exists

get_extension(*point: str, name: str*) \rightarrow Optional[*xcube.util.extension*.*Extension*] Get registered extension for given *point* and *name*.

Parameters

- **point** (str) extension point identifier
- **name** (str) extension name

Returns the extension or None, if no such exists

get_component(point: str, name: str) \rightarrow Any

Get extension component for given point and name. Raises a ValueError if no such extension exists.

Parameters

- **point** (str) extension point identifier
- **name** (str) extension name

Returns extension component

find_extensions(*point: str, predicate: Optional[Callable[[xcube.util.extension.Extension], bool]]* = None) \rightarrow List[*xcube.util.extension.Extension*]

Find extensions for *point* and optional filter function *predicate*.

The filter function is called with an extension and should return a truth value to indicate a match or mismatch.

Parameters

- **point** (str) extension point identifier
- predicate optional filter function

Returns list of matching extensions

find_components(*point: str, predicate: Optional[Callable[[*xcube.util.extension.Extension], *bool]]* = None) \rightarrow List[Any]

Find extension components for *point* and optional filter function *predicate*.

The filter function is called with an extension and should return a truth value to indicate a match or mismatch.

Parameters

- **point** (str) extension point identifier
- predicate optional filter function

Returns list of matching extension components

```
add_extension(point: str, name: str, component: Optional[Any] = None, loader:
```

Optional[*Callable*[[xcube.util.extension.Extension], *Any*]] = *None*, ***metadata*) \rightarrow *xcube.util.extension*.*Extension*

Register an extension *component* or an extension component *loader* for the given extension *point*, *name*, and additional *metadata*.

Either component or loader must be specified, but not both.

A given *loader* must be a callable with one positional argument *extension* of type *Extension* and is expected to return the actual extension component, which may be of any type. The *loader* will only be called once and only when the actual extension component is requested for the first time. Consider using the function *import_component()* to create a loader that lazily imports a component from a module and optionally executes it.

Return type *Extension*

Parameters

- **point** (str) extension point identifier
- **name** (str) extension name
- **component** extension component
- **loader** extension component loader function
- metadata extension metadata

Returns a registered extension

remove_extension(point: str, name: str)

Remove registered extension name from given point.

Parameters

- **point** (str) extension point identifier
- **name** (str) extension name

to_dict()

Get a JSON-serializable dictionary representation of this extension registry.

An extension that provides a component of any type.

Extensions are registered in a *ExtensionRegistry*.

Extension objects are not meant to be instantiated directly. Instead, *ExtensionRegistry.add_extension()* is used to register extensions.

Parameters

- **point** extension point identifier
- **name** extension name
- **component** extension component
- loader extension component loader function
- **metadata** extension metadata

property is_lazy: bool Whether this is a lazy extension that uses a loader.

property component: Any

Extension component.

property point: str Extension point identifier.

property name: str Extension name.

property metadata: Dict[str, Any]

Extension metadata.

 $to_dict() \rightarrow Dict[str, Any]$ Get a JSON-serializable dictionary representation of this extension.

xcube.util.extension.import_component(spec: str, transform: Optional[Callable[[Any,

xcube.util.extension.Extension], Any]] = None, call: bool = False, call_args: Optional[Sequence[Any]] = None, call_kwargs: Optional[Mapping[str, Any]] = None) \rightarrow Callable[[xcube.util.extension.Extension], Any]

Return a component loader that imports a module or module component from *spec*. To import a module, *spec* should be the fully qualified module name. To import a component, *spec* must also append the component name to the fully qualified module name separated by a color (":") character.

An optional *transform* callable my be used to transform the imported component. If given, a new component is computed:

component = transform(component, extension)

If the *call* flag is set, the component is expected to be a callable which will be called using the given *call_args* and *call_kwargs* to produce a new component:

component = component(*call_kwargs, **call_kwargs)

Finally, the component is returned.

Parameters

- **spec** (str) String of the form "module_path" or "module_path:component_name"
- **transform** callable that takes two positional arguments, the imported component and the extension of type *Extension*
- **call** (bool) Whether to finally call the component with given *call_args* and *call_kwargs*
- call_args arguments passed to a callable component if call flag is set
- call_kwargs keyword arguments passed to callable component if call flag is set

Returns a component loader

- xcube.constants.EXTENSION_POINT_INPUT_PROCESSORS = 'xcube.core.gen.iproc'
 The extension point identifier for input processor extensions
- xcube.constants.EXTENSION_POINT_DATASET_IOS = 'xcube.core.dsio'
 The extension point identifier for dataset I/O extensions
- xcube.constants.EXTENSION_POINT_CLI_COMMANDS = 'xcube.cli'
 The extension point identifier for CLI command extensions
- xcube.util.plugin.get_extension_registry() \rightarrow xcube.util.extension.ExtensionRegistry Get populated extension registry.
- xcube.util.plugin.get_plugins() \rightarrow Dict[str, Dict] Get mapping of "xcube_plugins" entry point names to JSON-serializable plugin meta-information.

CHAPTER

WEB API AND SERVER

xcube's RESTful web API is used to publish data cubes to clients. Using the API, clients can

- List configured xcube datasets;
- Get xcube dataset details including metadata, coordinate data, and metadata about all included variables;
- Get cube data;
- Extract time-series statistics from any variable given any geometry;
- Get spatial image tiles from any variable;
- Browse datasets and retrieve dataset data and metadata using the STAC API;
- Get places (GeoJSON features including vector data) that can be associated with xcube datasets.

Later versions of API will also allow for xcube dataset management including generation, modification, and deletion of xcube datasets.

The complete description of all available functions is provided via openapi.html after starting the server locally. Please check out *Publishing xcube datasets* to learn how to do access it.

The web API is provided through the *xcube server* which is started using the *xcube serve* CLI command.

CHAPTER

SEVEN

VIEWER APP

The xcube viewer app is a simple, single-page web application to be used with the xcube server.

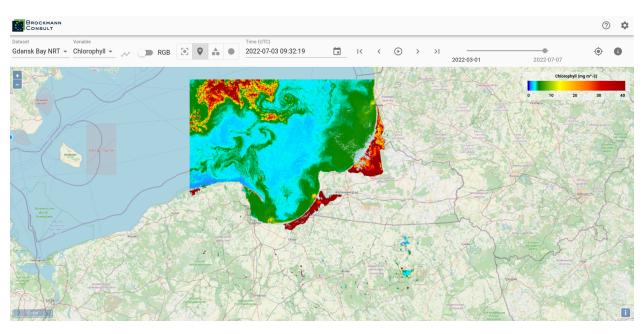
7.1 Demo

To test the viewer app, you can use the xcube viewer demo. This is our Brockmann Consult Demo xcube viewer. Via the viewer's settings it is possible to change the xcube server url which is used for displaying data. To do so open the viewer's settings panels, select "Server". A "Select Server" panel is opened, click the "+" button to add a new server. Here is demo server that you may add for testing:

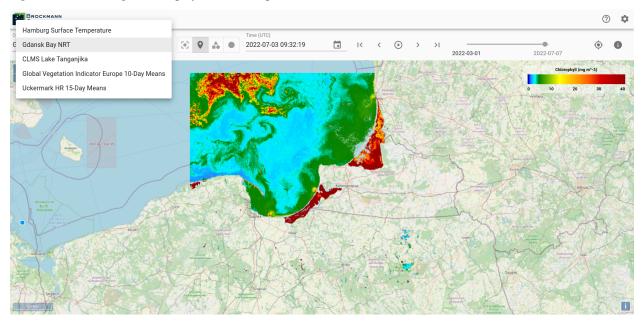
• Euro Data Cube Server (https://edc-api.brockmann-consult.de/api) has integrated amongst others a data cube with global essential climate variables (ECVs) variables from the ESA Earth System Data Lab Project. To access the Euro Data Cube viewer directly please visit https://edc-viewer.brockmann-consult.de.

7.2 Functionality

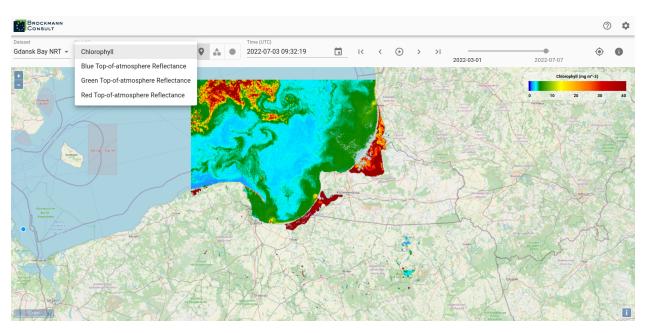
The xcube viewer functionality is described exemplary using the xcube viewer demo. The viewer visualizes data from the xcube datasets on top of a basemap. For zooming use the buttons in the top right corner of the map window or the zooming function of your computer mouse. A scale for the map is located in the lower right corner and in the upper left corner a corresponding legend to the mapped data of the data cube is available.



A xcube viewer may hold several xcube datasets which you can select via the drop-down menu *Dataset*. The viewed area automatically adjusts to a selected xcube dataset, meaning that if a newly selected dataset is located in a different region, the correct region is displayed on the map.



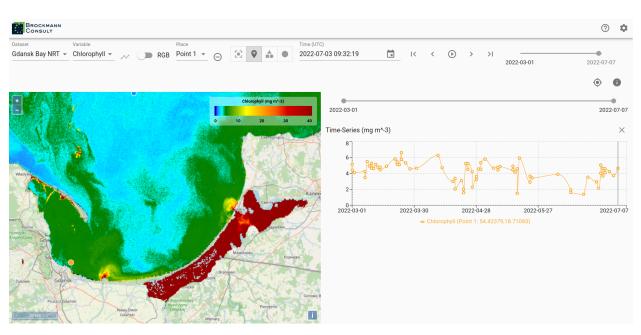
If more than one variable is available within a selected xcube dataset, you may change the variable by using the dropdown menu *Variable*.



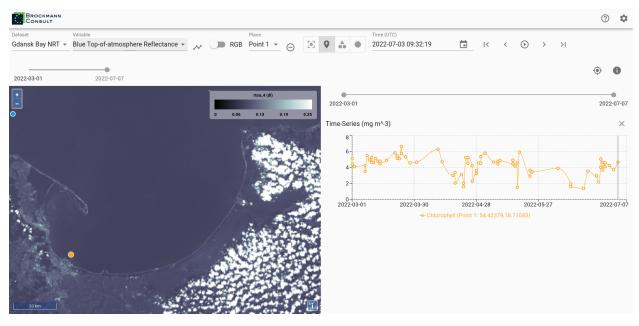
To see metadata for a dataset click on the *info*-icon on the right-hand side. Besides the dataset metadata you will see the metadata for the selected variable.

ROCKMANN Consult	0 🌣
Dataset Variable Place Place Circle 1 • O Image (UTC) 2022-04:3	22 09:37:54
	<u>ن</u>
Chorophyl (mg m-3)	1 1 * ? ×
0 10 20 30 40	Gdansk Bay NRT 🔳 🖒
	ID: bc-demo~Sweden/ws-s3-I2-gdansk-Sweden-v1.zarr
•	Dimension names lat, time, lon
	Dimension data types float64, datetime64[ns], float64
Denner A	Dimension lengths 1024, 273, 2048
Калининград	Geographical extent (x1, y1, x2, y2) 17.333333333333333333333333333333333333
	Spatial reference system EPSG:4326
	Chlorophyll Tr 🗉 <>
Asta Braniwo Earparonoeck -	Title Chlorophyll
Gdansk	Name Chlorophyll
Pruster Standal Before Standal Gorgeo Havestee	Units mg m^-3
Protect pourma 2 0 km Newy Dwor Extrational Cashtau Misocrymy EthopSur	Data type float32

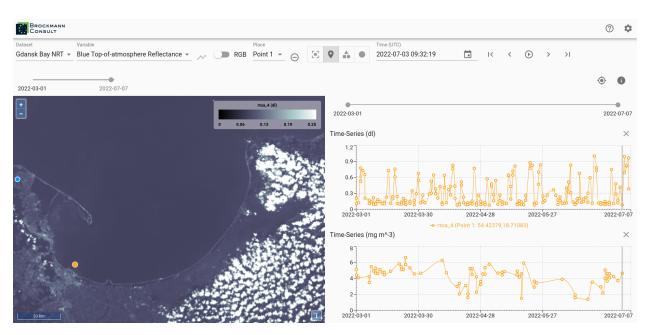
To obtain a time series set a point marker on the map and then select the *graph*-icon next to the *Variables* drop-down menu. You can select a different date by clicking into the time series graph on a value of interest. The data displayed in the viewer changes accordingly to the newly selected date.



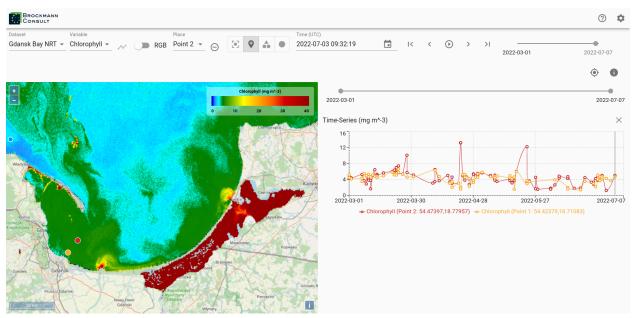
The current date is preserved when you select a different variable and the data of the variable is mapped for the date.



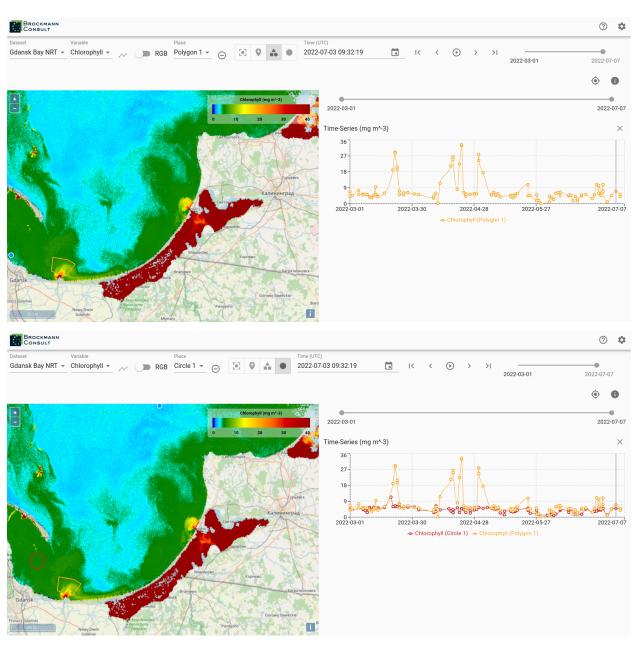
To generate a time series for the newly selected variable press the time series-icon again.



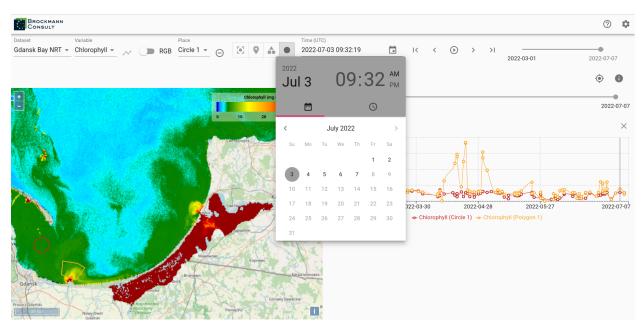
You may place multiple points on the map and you can generate time series for them. This allows a comparison between two locations. The color of the points corresponds to the color of the graph in the time series. You can find the coordinates of the point markers visualized in the time series beneath the graphs.



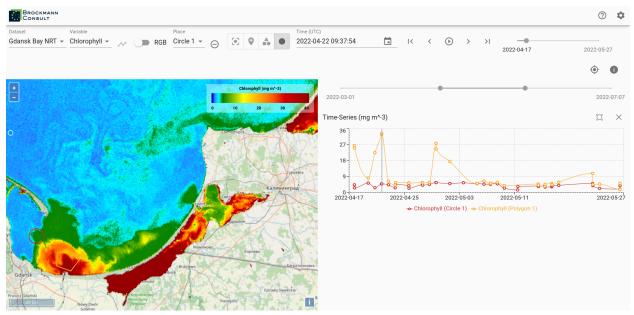
To delete a created location use the *remove*-icon next to the *Place* drop-down menu. Not only point location may be selected via the viewer, you can draw polygons and circular areas by using the icons on the right-hand side of the *Place* drop-down menu as well. You can visualize time series for areas, too.



In order to change the date for the data display use the calendar or step through the time line with the arrows on the right-hand side of the calendar.



When a time series is displayed two time-line tools are visible, the upper one for selecting the date displayed on the map of the viewer and the lower one may be used to narrow the time frame displayed in the time series graph. Just above the graph of the time series on the right-hand side is an *x*-icon for removing the time series from the view and to left of it is an icon which sets the time series back to the whole time extent.



To adjust the default settings select the *Settings*-icon on the very top right corner. There you have the possibility to change the server url, in order to view data which is available via a different server. You can choose a different language - if available - as well as set your preferences of displaying data and graph of the time series.

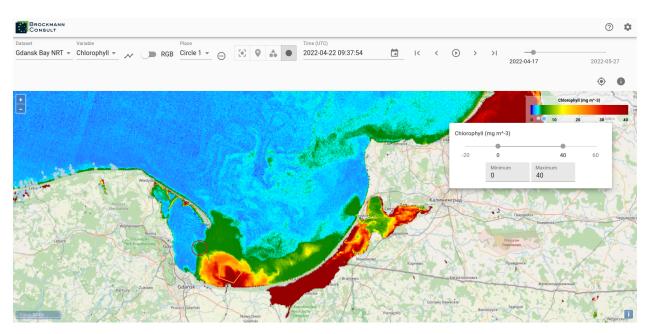
BROCKMANN						? 🌣
Dataset Gdansk Bay NRT →	Variable Chlorophyll - A RGB	Place Circle 1	Settings		>>>	
			General		2022-04-17	2022-05-27
+ o			Server BC DEMO Server			<u>ن</u>
		and and	Language English			2022-07-07
	and the second	i sente	Time interval of the player	1000 ms 👻		x Q
		10 Eggs.	Time-Series			
	t Reitig		Show graph after adding a place On	-	2	
A.			Show dots only, hide lines Off		2022-05-03 2022-05-11	2022-05-27
	and he		Show error bars On	-	II (Circle 1) Chlorophyll (Polygon 1)	
	1000 P	1	Show median instead of mean (disables error bars) On	-		
Gdansk		Branlewo	Minimal number of data points in a time series update	20		
Pruszcz Gdański	thicko	1.	Мар			
20 km	Nowy Dwór Griański	100	Base map			

To see the map settings please scroll down in the settings window. There you can adjust the base map, switch the displayed projection between *Geographic* and *Mercator*. You can also choose to turn image smoothing on and to view the dataset boundaries.

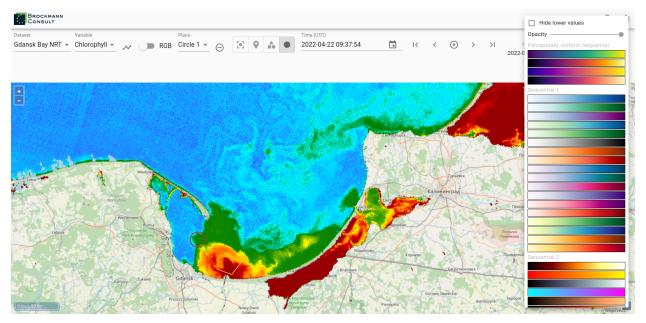
On the very bottom of the Settings pop-up window you can see information about the viewer and server version.

BROCKMANN	Show dots only, hide lines Off	> ()
Dataset Variable Place Gdansk Bay NRT Chlorophyll RGB Circle 1	Show error bars On	• > > <u>-</u> 2022-04-17 2022-05-27
	Show median instead of mean (disables error bars) On	• •
+ 0	Minimal number of data points in a time series update	2022-07-07
A State of the second sec	Мар	
and the second	Base map OpenStreetMap / OSM Mapnik	× ¤
	Projection Geographic O Merc	ator
	Image smoothing Off	
	Show dataset boundaries Off	2022-05-03 2022-05-11 2022-05-27 II (Circle 1) -> Chlorophyll (Polygon 1)
S Re La	System Information	
	xcube Viewer version 0.11.1	
Gans: may may	xcube Server version 0.11.2	
Prusez Bduński 20 km Nowy Dwár Gdański	Penietto	

Back to the general view, if you would like to change the value ranges of the displayed variable you can do it by clicking into the area of the legend where the value ticks are located or you can enter the desired values in the *Minimum* and/or *Maximum* text field.



You can change the color mapping as well by clicking into the color range of the legend. There you can also decide to hide lower values and it is possible to adjust the opacity.



The xcube viewer app is constantly evolving and enhancements are added, therefore please be aware that the above described features may not always be completely up-to-date.

7.3 Build and Deploy

You can also build and deploy your own viewer instance. In the latter case, visit the xcube-viewer repository on GitHub and follow the instructions provides in the related README file.

EIGHT

THE XCUBE GENERATOR

8.1 Introduction

The *generator* is an xcube feature which allows users to create, manipulate, and write xcube datasets according to a supplied configuration. The same configuration can be used to generate a dataset on the user's local computer or remotely, using an online server.

The generator offers two main user interfaces: A Python API, configured using Python objects; and a command-line interface, configured using YAML or JSON files. The Python and file-based configurations have the same structure and are interconvertible.

The online generator service interfaces with the xcube client via a well-defined REST API; it is also possible for thirdparty clients to make use of this API directly, though it is expected that the Python and command-line interfaces will be more convenient in most cases.

8.2 Further documentation

This document aims to provide a brief overview of the generation process and the available configuration options. More details are available in other documents and in the code itself:

- Probably the most thorough documentation is available in the Jupyter demo notebooks in the xcube repository. These can be run in any JupyterLab environment containing an xcube installation. They combine explanation with interactive worked examples to demonstrate practical usage of the generator in typical use cases.
- For the Python API in particular, the xcube API documentation is generated from the docstrings included in the code itself and serves as a detailed low-level reference for individual Python classes and methods. The docstrings can also be read from a Python environment (e.g. using the ? postfix in IPython or JupyterLab) or, of course, by browsing the source code itself.
- For the YAML/JSON configuration syntax used with the command-line interface, there are several examples available in the examples/gen2/configs subdirectory of the xcube repository.
- For the REST API underlying the Python and command-line interfaces, there is a formal definition on Swagger-Hub, and one of the example notebooks demonstrates its usage with the Python *requests* library.

8.3 The generation process

The usual cube generation process is as follows:

- 1. The generator opens the input data store using the store identifier and parameters in the *input configuration*.
- 2. The generator reads from the input store the data specified in the *cube configuration* and uses them to create a data cube, often with additional manipulation steps such as resampling the data.
- 3. If an optional *code configuration* has been given, the user-supplied code is run on the created data cube, potentially modifying it.
- 4. The generator writes the generated cube to the data store specified in the *output configuration*.

8.4 Invoking the generator from a Python environment

The configurations for the various parts of the generator are used to initialize a GeneratorRequest, which is then passed to xcube.core.gen2.generator.CubeGenerator.generate_cube. The generate_cube method returns a *cube reference* which can be used to open the cube from the output data store.

The generator can also be directly invoked with a configuration file from a Python environment, using the xcube. core.gen2.generator.CubeGenerator.from_file method.

8.5 Invoking the generator from the command line

The generator can be invoked from the command line using the xcube gen2 subcommand. (Note: the subcommand xcube gen invokes an earlier, deprecated generator feature which is not compatible with the generator framework described here.)

8.6 Configuration syntax

All Python configuration classes are defined in the xcube.core.gen2 package, except for CodeConfig, which is in xcube.core.byoa.

The types in the parameter tables are given in an ad-hoc, semi-formal notation whose corresponding Python and JSON representations should be obvious. For the formal Python type definitions, see the signatures of the __init__ methods of the configuration classes; for the formal JSON type definitions, see the JSON schemata (in JSON Schema format) produced by the get_schema methods of the configuration classes.

8.6.1 Remote generator service configuration

The command-line interface allows a *service configuration* for the remote generator service to be provided as a YAML or JSON file. This file defines the endpoint and access credentials for an online generator service. If it is provided, the specified remote service will be used to generate the cube. If it is omitted, the cube will be generated locally. The configuration file defines three values: endpoint_url, client_id, and client_secret. A typical service configuration YAML file might look as follows:

```
endpoint_url: "https://xcube-gen.brockmann-consult.de/api/v2/"
client_id: "93da366d7c39517865e4f141ddf1dd81"
client_secret: "d210aG91dCByZXN0cmljdGlvbiwgaW5jbHVkaW5nIHd"
```

8.6.2 Store configuration

In the command-line interface, an additional YAML or JSON file containing one or more *store configurations* may be supplied. A store configuration encapsulates a data store ID and an associated set of store parameters, which can then be referenced by an associated *store configuration identifier*. This identifier can be used in the input configuration, as described below. A typical YAML store configuration might look as follows:

```
sentinelhub_eu:
  title: SENTINEL Hub (Central Europe)
  description: Datasets from the SENTINEL Hub API deployment in Central Europe
  store id: sentinelhub
  store_params:
    api_url: https://services.sentinel-hub.com
    client_id: myid123
    client_secret: 0c5892208a0a82f1599df026b5e19017
cds:
  title: C3S Climate Data Store (CDS)
  description: Selected datasets from the Copernicus CDS API
  store_id: cds
  store_params:
   normalize_names: true
   num retries: 3
my_data_bucket:
  title: S3 output bucket
  description: An S3 bucket for output data sets
  store id: s3
  store_params:
   root: cube-outputs
    storage_options:
      key: qwerty12345
      secret: 7ff889c0aea254d5e00440858289b85c
      client_kwargs:
        endpoint_url: https://my-endpoint.some-domain.org/
```

8.6.3 Input configuration

The input configuration defines the data store from which data for the cube are to be read, and any additional parameters which this data store requires.

The Python configuration object is InputConfig; the corresponding YAML configuration section is input_configs.

Parameter	Required?	Туре	Description
store_id	N	str	Identifier for the data store
opener_id	N	str	Identifier for the data opener
data_id	Y	str	Identifier for the dataset
store_params	N	$map(str \rightarrow *)$	Parameters for the data store
open_params	N	$map(str \rightarrow *)$	Parameters for the data opener

store_id is a string identifier for a particular xcube data store, defined by the data store itself. If a store configuration file has been supplied (see above), a store configuration identifier can also be supplied here in place of a 'plain' store identifier. Store configuration identifiers must be prefixed by an @ symbol. If a store configuration identifier is supplied

in place of a store identifier, store_params values will be supplied from the predefined store configuration and can be omitted from the input configuration.

data_id is a string identifier for the dataset within a particular store.

The format and content of the store_params and open_params dictionaries is defined by the individual store or opener.

The generator service does not yet provide a remote interface to list available data stores, datasets, and store parameters (i.e. allowed values for the parameters in the table above). In a local xcube Python environment, you can list the currently available store identifiers with the expression list(map(lambda e: e.name, xcube.core.store.find_data_store_extensions())). You can create a local store object for an identifier store_id with xcube.core.store.get_data_store_instance(store_id).store. The store object provides methods list_data_ids, get_data_store_params_schema, and get_open_data_params_schema to describe the allowed values for the corresponding parameters. Note that the available stores and datasets on a remote xcube generator server may not be the same as those available in your local xcube environment.

8.6.4 Cube configuration

This configuration element defines the characteristics of the cube that should be generated. The Python configuration class is called CubeConfig, and the YAML section cube_config. All parameters are optional and will be filled in with defaults if omitted; the default values are dependent on the data store and dataset.

Parameter	Туре	Units/Description	
<pre>variable_names[str,]</pre>		Available variables are data store dependent.	
crs	str	PROJ string, JSON string with PROJ parameters, CRS WKT string, or	
		authority string	
bbox	[float, float, float,	Bounding-box (min_x, min_y, max_x, max_y) CRS-dependent, usually	
	float]	degrees	
spatial_res	float or [float, float]	CRS-dependent, usually degrees	
tile_size	int or [int, int]	pixels	
time_range	str or [str, str]	ISO 8601 subset	
time_period	str	integer + unit	
chunks	map(str→null/int)	maps variable names to chunk sizes	

The crs parameter string is interpreted using `CRS.from_string in the pyproj package <https://pyproj4.github.io/ pyproj/dev/api/crs/crs.html#pyproj.crs.CRS.from_string>`___ and therefore accepts the same specifiers.

time_range specified the start and end of the requested time range. can be specified either as a date in the format YYYY-MM-DD or as a date and time in the format YYYY-MM-DD HH:MM:SS. If the time is omitted, it is taken to be 00:00:00 (the start of the day) for the start specifier and 24:00:00 (the end of the day) for the specifier. The end specifier may be omitted; in this case the current time is used.

time_period specified the duration of a single time step in the requested cube, which determines the temporal resolution. It consists of an integer denoting the number of time units, followed by single upper-case letter denoting the time unit. Valid time unit specifiers are D (day), W (week), M (month), and Y (year). Examples of time_period values: 1Y (one year), 2M (two months), 10D (ten days).

The value of the chunks mapping determines how the generated data is chunked for storage. The chunking has no effect on the data itself, but can have a dramatic impact on data access speeds in different scenarios. The value of chunks is structured a map from variable names (corresponding to those specified by the variable_names parameter) to chunk sizes.

8.6.5 Code configuration

The code configuration supports multiple ways to define a *dataset processor* – fundamentally, a Python function which takes a dataset and returns a processed version of the input dataset. Since the code configuration can work directly with instantiated Python objects (which can't be stored in a YAML file), there are some differences in code configuration between the Python API and the YAML format.

Parameter	Туре	Units/description
_callable †	Callable	Function to be called to process the datacube. Only available via
		Python API
callable_ref	str (non-empty)	A reference to a Python class or function, in the format <module>:<</module>
		<pre>function_or_class></pre>
callable_para	m s nap(str→*)	Parameters to be passed to the specified callable
inline_code	str (non-empty)	An inline snippet of Python code
†		
file_set †	FileSet (Python) / map	A bundle of Python modules or packages (see details below)
	(YAML)	
install_requir ed olean		If set, indicates that file_set contains modules or packages to be
		installed.

All parameters are optional (as is the entire code configuration itself). The three parameters marked † are mutually exclusive: at most one of them may be given.

_callable provides the dataset processor directly and is only available in the Python API. It must be either a function or a class.

- If a function, it takes a Dataset and optional additional named parameters, and returns a Dataset. Any additional parameters are supplied in the callable_params parameter of the code configuration.
- If an object, it must implement a method process_dataset, which is treated like the function described above, and may optionally implement a class method get_process_params_schema, which returns a JsonObjectSchema describing the additional parameters. For convenience and clarity, the object may extend the abstract base class DatasetProcessor, which declares both these methods.

callable_ref is a string with the structure <module>:<function_or_class>, and specifies the function or class to call when inline_code or file_set is provided. The specified function or class is handled like the _callable parameter described above.

callable_params specifies a dictionary of named parameters which are passed to the processor function or method.

inline_code is a string containing Python source code. If supplied, it should contain the definition of a function or object as described for the _callable parameter. The module and class identifiers for the callable in the inline code snippet should be specified in callable_ref parameter.

file_set specifies a set of files which should be read from an fsspec file system and which contain a definition of a dataset processor. As with inline_code, the parameter callable_ref should also be supplied to tell the generator which class or function in the file set is the actual processor. The parameters of file_set are identical with those of the constructor of the corresponding Python FileSet class, and are as follows:

Parameter	Туре	Description
path	str	fsspec-compatible root path specifier
sub_path	str	optional sub-path to append to main path
includes	[str]	include files matching any of these patterns
excludes	[str]	exclude files matching any of these patterns
storage_params	$map(str \rightarrow *)$	FS-specific parameters (passed to fsspec)

8.6.6 Output configuration

This configuration element determines where the generated cube should be written to. The Python configuration class is called OutputConfig, and the YAML section output_config.

Parameter	Туре	Units/description
store_id	str	Identifier of output store
writer_id	str	Identifier of data writer
data_id	str	Identifier under which to write the cube
store_params	$map(str \rightarrow *)$	Store-dependent parameters for output store
write_params	$map(str \rightarrow *)$	Writer-dependent parameters for output writer
replace	bool	If true, replace any existing data with the same identifier.

NINE

XCUBE DATASET SPECIFICATION

This document provides a technical specification of the protocol and format for *xcube datasets*, data cubes in the xcube sense.

The key words "MUST", "MUST NOT", "REQUIRED", "SHALL", "SHALL NOT", "SHOULD", "SHOULD NOT", "RECOMMENDED", "MAY", and "OPTIONAL" in this document are to be interpreted as described in RFC 2119.

9.1 Document Status

This is the latest version, which is still in development.

Version: 1.0, draft

Updated: 31.05.2018

9.2 Motivation

For many users of Earth observation data, multivariate coregistration, extraction, comparison, and analysis of different data sources is difficult, while data is provided in various formats and at different spatio-temporal resolutions.

9.3 High-level requirements

xcube datasets

- SHALL be time series of gridded, geo-spatial, geo-physical variables.
- SHALL use a common, equidistant, global or regional geo-spatial grid.
- SHALL shall be easy to read, write, process, generate.
- SHALL conform to the requirements of analysis ready data (ARD).
- SHALL be compatible with existing tools and APIs.
- SHALL conform to standards or common practices and follow a common data model.
- SHALL be formatted as self-contained datasets.
- SHALL be "cloud ready", in the sense that subsets of the data can be accessed by individual URIs.

ARD links:

http://ceos.org/ard/

- https://landsat.usgs.gov/ard
- https://medium.com/planet-stories/analysis-ready-data-defined-5694f6f48815

9.4 xcube Dataset Schemas

9.4.1 Basic Schema

- Attributes metadata convention
 - SHALL be CF >= 1.7
 - SHOULD adhere to Attribute Convention for Data Discovery
- Dimensions:
 - SHALL be at least time, bnds, and MAY be any others.
 - SHALL all be greater than zero, but bnds must always be two.
- Temporal coordinate variables:
 - SHALL provide time coordinates for given time index.
 - MAY be non-equidistant or equidistant.
 - time[time] SHALL provide observation or average time of *cell centers*.
 - time_bnds[time, bnds] SHALL provide observation or integration time of *cell boundaries*.
 - Attributes:
 - * Temporal coordinate variables MUST have units, standard_name, and any others.
- Spatial coordinate variables
 - SHALL provide spatial coordinates for given spatial index.
 - SHALL be equidistant in either angular or metric units
- Cube variables:
 - SHALL provide *cube cells* with the dimensions as index.
 - SHALL have shape
 - * [time, ..., lat, lon] (see WGS84 schema) or
 - * [time, ..., y, x] (see Generic schema)
 - MAY have extra dimensions, e.g. layer (of the atmosphere), band (of a spectrum).
 - SHALL specify the units metadata attribute.
 - SHOULD specify metadata attributes that are used to identify missing values, namely _FillValue and / or valid_min, valid_max, see notes in CF conventions on these attributes.
 - MAY specify metadata attributes that can be used to visualise the data:
 - * color_bar_name: Name of a predefined colour mapping. The colour bar is applied between a minimum and a maximum value.

* color_value_min, color_value_max: Minimum and maximum value for applying the colour bar. If not provided, minimum and maximum default to valid_min, valid_max. If neither are provided, minimum and maximum default to 0 and 1.

9.4.2 WGS84 Schema (extends Basic)

- Dimensions:
 - SHALL be at least time, lat, lon, bnds, and MAY be any others.
- Spatial coordinate variables:
 - SHALL use WGS84 (EPSG:4326) CRS.
 - SHALL have lat[lat] that provides observation or average latitude of *cell centers* with attributes: standard_name="latitude" units="degrees_north".
 - SHALL have lon[lon] that provides observation or average longitude of *cell centers* with attributes: standard_name="longitude" and units="degrees_east".
 - SHOULD HAVE lat_bnds[lat, bnds], lon_bnds[lon, bnds]: provide geodetic observation or integration coordinates of *cell boundaries*.
- Cube variables:
 - SHALL have shape [time, ..., lat, lon].

9.4.3 Generic Schema (extends Basic)

- Dimensions: time, y, x, bnds, and any others.
 - SHALL be at least time, y, x, bnds, and MAY be any others.
- Spatial coordinate variables:
 - Any spatial grid and CRS.
 - y[y], x[x]: provide spatial observation or average coordinates of *cell centers*.
 - * Attributes: standard_name, units, other units describe the CRS / projections, see CF.
 - y_bnds[y, bnds], x_bnds[x, bnds]: provide spatial observation or integration coordinates of *cell boundaries*.
 - MAY have lat[y,x]: latitude of *cell centers*.
 - * Attributes: standard_name="latitude", units="degrees_north".
 - lon[y,x]: longitude of *cell centers*.
 - * Attributes: standard_name="longitude", units="degrees_east".
- Cube variables:
 - MUST have shape [time, \dots , y, x].

9.5 xcube EO Processing Levels

This section provides an attempt to characterize xcube datasets generated from Earth Observation (EO) data according to their processing levels as they are commonly used in EO data processing.

9.5.1 Level-1C and Level-2C

- Generated from Level-1A, -1B, -2A, -2B EO data.
- Spatially resampled to common grid
 - Typically resampled at original resolution.
 - May be down-sampled: aggregation/integration.
 - May be upsampled: interpolation.
- No temporal aggregation/integration.
- Temporally non-equidistant.

9.5.2 Level-3

- Generated from Level-2C or -3 by temporal aggregation.
- No spatial processing.
- Temporally equidistant.
- Temporally integrated/aggregated.

TEN

XCUBE DEVELOPER GUIDE

Version 0.2, draft

IMPORTANT NOTE: Any changes to this doc must be reviewed by dev-team through pull requests.

10.1 Table of Contents

- Versioning
- Coding Style
- Main Packages
 - Package xcube.core
 - Package xcube.cli
 - Package xcube.webapi
 - Package xcube.util
- Development Process

10.2 Versioning

We adhere to PEP-440. Therefore, the xcube software version uses the format <major>.<micro> for released versions and <major>.<micro>.dev<n> for versions in development.

- <major> is increased for major enhancements. CLI / API changes may introduce incompatibilities with former version.
- <minor> is increased for new features and and minor enhancements. CLI / API changes are backward compatible with former version.
- <micro> is increased for bug fixes and micro enhancements. CLI / API changes are backward compatible with former version.
- <n> is increased whenever the team (internally) deploys new builds of a development snapshot.

The current software version is in xcube/version.py.

10.3 Coding Style

We follow PEP-8, including its recommendation of PEP-484 syntax for type hints.

10.3.1 Updating code style in the existing codebase

A significant portion of the existing codebase does not adhere to our current code style guidelines. It is of course a goal to bring these parts into conformance with the style guide, but major style changes should not be bundled into pull requests focused on other improvements or bug fixes, because they obscure the significant code changes and make reviews difficult. Large-scale style and formatting updates should instead be made via dedicated pull requests.

10.3.2 Line length

As recommended in PEP-8, all lines should be limited to a maximum of 79 characters, including docstrings and comments.

10.3.3 Quotation marks for string literals

In general, single quotation marks should always be used for string literals. Double quotation marks should only be used if there is a compelling reason to do so in a particular case.

10.4 Main Packages

- xcube.core Hosts core API functions. Code in here should be maintained w.r.t. backward compatibility. Therefore think twice before adding new or change existing core API.
- xcube.cli Hosts CLI commands. CLI command implementations should be lightweight. Move implementation code either into core or util.CLI commands must be maintained w.r.t. backward compatibility. Therefore think twice before adding new or change existing CLI commands.
- xcube.webapi Hosts Web API functions. Web API command implementations should be lightweight. Move implementation code either into core or util.Web API interface must be maintained w.r.t. backward compatibility. Therefore think twice before adding new or change existing web API.
- xcube.util Mainly implementation helpers. Comprises classes and functions that are used by cli, core, webapi in order to maximize modularisation and testability but to minimize code duplication. The code in here must not be dependent on any of cli, core, webapi. The code in here may change often and in any way as desired by code implementing the cli, core, webapi packages.

The following sections will guide you through extending or changing the main packages that form xcube's public interface.

10.4.1 Package xcube.cli

Checklist

Make sure your change

- 1. is covered by unit-tests (package test/cli);
- 2. is reflected by the CLI's doc-strings and tools documentation (currently in README.md);
- 3. follows existing xcube CLI conventions;
- 4. follows PEP8 conventions;
- 5. is reflected in API and WebAPI, if desired;
- 6. is reflected in CHANGES.md.

Hints

Make sure your new CLI command is in line with the others commands regarding command name, option names, as well as metavar arguments names. The CLI command name shall ideally be a verb.

Avoid introducing new option arguments if similar options are already in use for existing commands.

In the following common arguments and options are listed.

Input argument:

```
@click.argument('input')
```

If input argument is restricted to an xcube dataset:

```
@click.argument('cube')
```

Output (directory) option:

Output format:

Output parameters:

Variable names:

For parsing CLI inputs, use helper functions that are already in use. In the CLI command implementation code, raise click.ClickException(message) with a clear message for users.

Common xcube CLI options like -f for FORMAT should be lower case letters and specific xcube CLI options like -S for SIZE in xcube gen are recommended to be uppercase letters.

Extensively validate CLI inputs to avoid that API functions raise ValueError, TypeError, etc. Such errors and their message texts are usually hard to understand by users. They are actually dedicated to to developers, not CLI users.

There is a global option --traceback flag that user can set to dump stack traces. You don't need to print stack traces from your code.

10.4.2 Package xcube.core

Checklist

Make sure your change

- 1. is covered by unit-tests (package test/core);
- 2. is covered by API documentation;
- 3. follows existing xcube API conventions;
- 4. follows PEP8 conventions;
- 5. is reflected in xarray extension class xcube.core.xarray.DatasetAccessor;
- 6. is reflected in CLI and WebAPI if desired;
- 7. is reflected in CHANGES.md.

Hints

Create new module in xcube.core and add your functions. For any functions added make sure naming is in line with other API. Add clear doc-string to the new API. Use Sphinx RST format.

Decide if your API methods requires *xcube datasets* as inputs, if so, name the primary dataset argument cube and add a keyword parameter cube_asserted: bool = False. Otherwise name the primary dataset argument dataset.

Reflect the fact, that a certain API method or function operates only on datasets that conform with the xcube dataset specifications by using cube in its name rather than dataset. For example compute_dataset can operate on any xarray datasets, while get_cube_values_for_points expects a xcube dataset as input or read_cube ensures it will return valid xcube datasets only.

In the implementation, if not cube_asserted, we must assert and verify the cube is a cube. Pass True to cube_asserted argument of other API called later on:

```
from xcube.core.verify import assert_cube

def frombosify_cube(cube: xr.Dataset, ..., cube_asserted: bool = False):
    if not cube_asserted:
        assert_cube(cube)
    ...
    result = bibosify_cube(cube, ..., cube_asserted=True)
    ...
```

If import xcube.core.xarray is imported in client code, any xarray.Dataset object will have an extra property xcube whose interface is defined by the class xcube.core.xarray.DatasetAccessor. This class is an xarray extension that is used to reflect xcube.core functions and make it directly applicable to the xarray.Dataset object.

Therefore any xcube API shall be reflected in this extension class.

10.4.3 Package xcube.webapi

Checklist

Make sure your change

- 1. is covered by unit-tests (package test/webapi);
- 2. is covered by Web API specification and documentation (currently in webapi/res/openapi.yml);
- 3. follows existing xcube Web API conventions;
- 4. follows PEP8 conventions;
- 5. is reflected in CLI and API, if desired;
- 6. is reflected in CHANGES.md.

10.4.4 Hints

- The Web API is defined in webapi.app which defines mapping from resource URLs to handlers
- All handlers are implemented in webapi.handlers. Handler code just delegates to dedicated controllers.
- All controllers are implemented in webapi.controllers.*. They might further delegate into core.*

10.5 Development Process

- 1. Make sure there is an issue ticket for your code change work item
- 2. Select issue, priorities are as follows
 - 1. "urgent" and ("important" and "bug")
 - 2. "urgent" and ("important" or "bug")
 - 3. "urgent"
 - 4. "important" and "bug"
 - 5. "important" or "bug"
 - 6. others
- 3. Make sure issue is assigned to you, if unclear agree with team first.
- 4. Add issue label "in progress".
- 5. Create development branch named "<developer>-<issue>-<title>" (see below).
- 6. Develop, having in mind the checklists and implementation hints above.
 - 1. In your first commit, refer the issue so it will appear as link in the issue history
 - 2. Develop, test, and push to the remote branch as desired.
 - 3. In your last commit, utilize checklists above. (You can include the line "closes #<issue>" in your commit message to auto-close the issue once the PR is merged.)
- 7. Create PR if build servers succeed on your branch. If not, fix issue first.For the PR assign the team for review, agree who is to merge. Also reviewers should have checklist in mind.
- 8. Merge PR after all reviewers are accepted your change. Otherwise go back.

- 9. Remove issue label "in progress".
- 10. Delete the development branch.
- 11. If the PR is only partly solving an issue:
 - 1. Make sure the issue contains a to-do list (checkboxes) to complete the issue.
 - 2. Do not include the line "closes #<issue>" in your last commit message.
 - 3. Add "relates to issue#" in PR.
 - 4. Make sure to check the corresponding to-do items (checkboxes) after the PR is merged.
 - 5. Remove issue label "in progress".
 - 6. Leave issue open.

10.6 Branches and Releases

10.6.1 Target Branch

The master branch contains latest developments, including new features and fixes. Its software version string is always <major>.<minor>.<micro>.dev<n>. The branch is used to generate major, minor, or maintenance releases. That is, either <major>, <minor>, or <fix> is increased. Before a release, the last thing we do is to remove the .dev<n> suffix, after a release, the first thing we do is to increase the micro version and add the .dev<n> suffix.

10.6.2 Development Branches

Development branches should be named <developer>-<issue>-<title> where

- <developer> is the github name of the code author
- <issue> is the number of the issue in the github issue tracker that is targeted by the works on this branch
- <title> is either the name of the issue or an abbreviated version of it

10.7 Release Process

10.7.1 Release on GitHub

This describes the release process for xcube. For a plugin release, you need to adjust the paths accordingly.

- Check issues in progress, close any open issues that have been fixed.
- Make sure that all unit tests pass and that test coverage is 100% (or as near to 100% as practicable).
- In xcube/version.py remove the .dev suffix from version name.
- Adjust version in Dockerfile accordingly.
- Make sure CHANGES.md is complete. Remove the suffix (in development) from the last version headline.
- Push changes to either master or a new maintenance branch (see above).
- Await results from Travis CI and ReadTheDocs builds. If broken, fix.
- Go to xcube/releases and press button "Draft a new Release".

- Tag version is: v\${version} (with a "v" prefix)
- Release title is: **\${version}** (without a "v" prefix)
- Paste latest changes from CHANGES.md into field "Describe this release"
- Press "Publish release" button
- After the release on GitHub, rebase sources, if the branch was master, create a new maintenance branch (see above)
- In xcube/version.py increase version number and append a .dev0 suffix to the version name so that it is still PEP-440 compatible.
- Adjust version in Dockerfile accordingly.
- In CHANGES.md add a new version headline and attach (in development) to it.
- Push changes to either master or a new maintenance branch (see above).
- Activate new doc version on ReadTheDocs.

Go through the same procedure for all xcube plugin packages dependent on this version of xcube.

10.7.2 Release on Conda-Forge

These instructions are based on the documentation at conda-forge.

Conda-forge packages are produced from a github feedstock repository belonging to the conda-forge organization. A repository's feedstock is usually located at https://github.com/conda-forge/<repo-name>-feedstock, e.g., https://github.com/conda-forge/xcube-feedstock. The package is updated by

- · forking the repository
- creating a new branch for the changes
- creating a pull request to merge this branch into conda-forge's feedstock repository (this is done automatically if the build number is 0).

The first of these steps is usually already done. You may find forks at https://github.com/dcs4cop/ <repo-name>-feedstock.

In detail, the steps are:

- 1. Update the dcs4cop fork of the feedstock repository, if it's not already up to date with conda-forge's upstream repository.
- 2. Clone the repository locally and create a new branch. The name of the branch is not strictly prescribed, but it's sensible to choose an informative name like update_ 0_5_3 .
- 3. In case the build number is 0, a bot will render the feedstock during the pull request. Otherwise, conduct the following steps: Rerender the feedstock using conda-smithy. This updates common conda-forge feedstock files. It's probably easiest to install conda-smithy in a fresh environment for this:

conda install -c conda-forge conda-smithy

conda smithy rerender -c auto

- 4. Update recipe/meta.yaml for the new version. Mainly this will involve the following steps:
 - 1. Update the value of the version variable (or, if the version number has not changed, increment the build number).
 - 2. If the version number has changed, ensure that the build number is set to 0.
 - 3. Update the sha256 hash of the source archive prepared by GitHub.

- 4. If the dependencies have changed, update the list of dependencies in the **-run** subsection to match those in the environment.yml file.
- 5. Commit the changes and push them to GitHub. A pull request at the feedstock repository on conda-forge will be automatically created by a bot if the build number is 0. If it is higher, you will have to create the pull request yourself.
- 6. Once conda-forge's automated checks have passed, merge the pull request.
- 7. Merge the newly-merged changes from the master branch on conda-forge back to the master branch of the dcs4cop fork. This step is not necessarily needed for the release, but it helps to avoid messy parallel branches.

Once the pull request has been merged, the updated package should usually become available from conda-forge within a couple of hours.

TODO: Describe deployment of xcube Docker image after release

If any changes apply to xcube serve and the xcube Web API:

Make sure changes are reflected in xcube/webapi/res/openapi.yml. If there are changes, sync xcube/webapi/res/openapi.yml with xcube Web API docs on SwaggerHub.

Check if changes affect the xcube-viewer code. If so make sure changes are reflected in xcube-viewer code and test viewer with latest xcube Web API. Then release a new xcube viewer.

10.7.3 xcube Viewer

- Cd into viewer project directory (.../xcube-viewer/.).
- Remove the -dev suffix from version property in package.json.
- Remove the -dev suffix from version constant in src/config.ts.
- Make sure CHANGES.md is complete. Remove the suffix (in development) from the last version headline.
- Build the app and test the build using a local http-server, e.g.:

\$ npm install -g http-server \$ cd build \$ http-server -p 3000 -c-1

- Push changes to either master or a new maintenance branch (see above).
- Goto xcube-viewer/releases and press button "Draft a new Release".
 - Tag version is: v\${version} (with a "v" prefix).
 - Release title is: \${version}.
 - Paste latest changes from CHANGES.md into field "Describe this release".
 - Press "Publish release" button.
- After the release on GitHub, if the branch was master, create a new maintenance branch (see above).
- Increase version property and version constant in package.json and src/config.ts and append -dev.0 suffix to version name so it is SemVer compatible.
- In CHANGES.md add a new version headline and attach (in development) to it.
- Push changes to either master or a new maintenance branch (see above).
- Deploy builds of master branches to related web content providers.

ELEVEN

PLUGINS

xcube's functionality can be extended by plugins. A plugin contributes extensions to specific extension points defined by xcube. Plugins are detected and dynamically loaded, once the available extensions need to be inquired.

11.1 Installing Plugins

Plugins are installed by simply installing the plugin's package into xcube's Python environment.

In order to be detected by xcube, an plugin package's name must either start with xcube_ or the plugin package's setup.py file must specify an entry point in the group xcube_plugins. Details are provided below in section *plu-gin_development*.

11.2 Available Plugins

11.2.1 SENTINEL Hub

The xcube_sh plugin adds support for the SENTINEL Hub Cloud API. It extends xcube by a new Python API function xcube_sh.cube.open_cube to create data cubes from SENTINEL Hub on-the-fly. It also adds a new CLI command xcube sh gen to generate and write data cubes created from SENTINEL Hub into the file system.

11.2.2 ESA CCI Open Data Portal

The xcube_cci plugin provides support for the ESA CCI Open Data Portal.

11.2.3 Copernicus Climate Data Store

The xcube_cds plugin provides support for the Copernicus Climate Data Store.

11.2.4 Cube Generation

xcube's GitHub organisation currently hosts a few plugins that add new *input processor* extensions (see below) to xcube's data cube generation tool *xcube gen*. They are very specific but are a good starting point for developing your own input processors:

- xcube_gen_bc adds new input processors for specific Ocean Colour Earth Observation products derived from the Sentinel-3 OLCI measurements.
- xcube_gen_rbins adds new input processors for specific Ocean Colour Earth Observation products derived from the SEVIRI measurements.
- xcube_gen_vito adds new input processors for specific Ocean Colour Earth Observation products derived from the Sentinel-2 MSI measurements.

11.3 Plugin Development

11.3.1 Plugin Definition

An xcube plugin is a Python package that is installed in xcube's Python environment. xcube can detect plugins either

- 1. by naming convention (more simple);
- 2. by entry point (more flexible).

By naming convention: Any Python package named xcube_<name> that defines a plugin *initializer function* named init_plugin either defined in xcube_<name>/plugin.py (preferred) or xcube_<name>/__init__.py is an xcube plugin.

By entry point: Any Python package installed using Setuptools that defines a non-empty entry point group xcube_plugins is an xcube plugin. An entry point in the xcube_plugins group has the format <name> = <fully-qualified-module-path>:<init-func-name>, and therefore specifies where plugin *initializer function* named <init-func-name> is found. As an example, refer to the xcube standard plugin definitions in xcube's setup.py file.

For more information on Setuptools entry points refer to section Creating and discovering plugins in the Python Packing User Guide and Dynamic Discovery of Services and Plugins in the Setuptools documentation.

11.3.2 Initializer Function

xcube plugins are initialized using a dedicated function that has a single *extension registry* argument of type *xcube*. *util.extension.ExtensionRegistry*, that is used by plugins's to register their extensions to xcube. By convention, this function is called init_plugin, however, when using entry points, it can have any name. As an example, here is the initializer function of the SENTINEL Hub plugin xcube_sh/plugin.py::

11.3.3 Extension Points and Extensions

When a plugin is loaded, it adds its extensions to predefined *extension points* defined by xcube. xcube defines the following extension points:

- xcube.core.gen.iproc: input processor extensions
- xcube.core.dsio: dataset I/O extensions
- xcube.cli: Command-line interface (CLI) extensions

An extension is added to the extension registry's add_extension method. The extension registry is passed to the plugin initializer function as its only argument.

11.3.4 Input Processor Extensions

Input processors are used the xcube gen CLI command and gen_cube API function. An input processor is responsible for processing individual time slices after they have been opened from their sources and before they are appended to or inserted into the data cube to be generated. New input processors are usually programmed to support the characteristics of specific xcube gen inputs, mostly specific Earth Observation data products.

By default, xcube uses a standard input processor named default that expects inputs to be individual NetCDF files that conform to the CF-convention. Every file is expected to contain a single spatial image with dimensions lat and lon and the time is expected to be given as global attributes.

If your input files do not conform with the default expectations, you can extend xcube and write your own input processor. An input processor is an implementation of the xcube.core.gen.iproc.InputProcessor or xcube. core.gen.iproc.XYInputProcessor class.

As an example take a look at the implementation of the default input processor xcube.core.gen.iproc.DefaultInputProcessor or the various input processor plugins mentioned above.

The extension point identifier is defined by the constant xcube.constants. EXTENSION_POINT_INPUT_PROCESSORS.

11.3.5 Dataset I/O Extensions

More coming soon...

The extension point identifier is defined by the constant xcube.constants.EXTENSION_POINT_DATASET_IOS.

11.3.6 CLI Extensions

CLI extensions enhance the xcube command-line tool by new sub-commands. The xcube CLI is implemented using the click library, therefore the extension components must be click commands or command groups.

The extension point identifier is defined by the constant xcube.constants.EXTENSION_POINT_CLI_COMMANDS.

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