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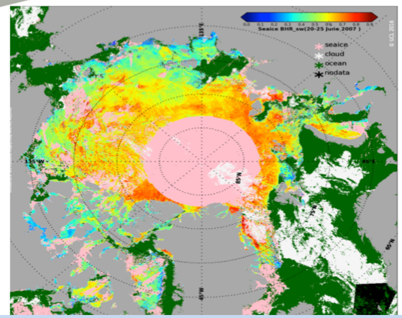

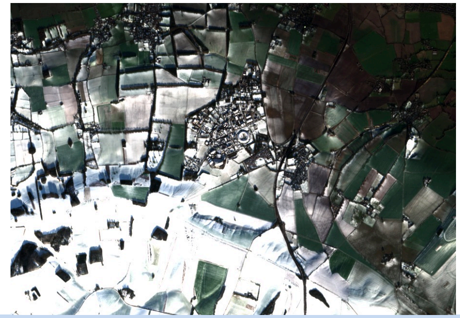

Semantic storage of climate data on object stores

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Abstract

s3-netCDF-python is a Python (and Cython) library that enables writing and reading netCDF files to and from any storage system that has an Amazon S3 API.

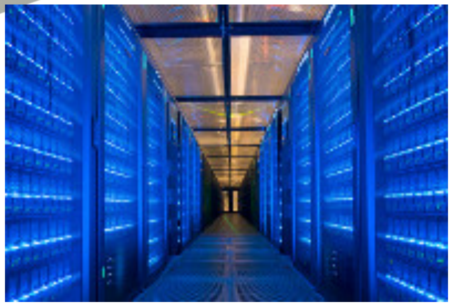
- S3 (simple storage solution) HTTP API used by
  - Object stores
  - Cloud-based storage (e.g. AWS)
- netCDF3 or netCDF4 (HDF5 based)
- netCDF file can be split into smaller “fragments”
  - Read only part(s) of the file that are required
  - Allow the parallel read and write of file fragments
  - Just-in-time reading and writing

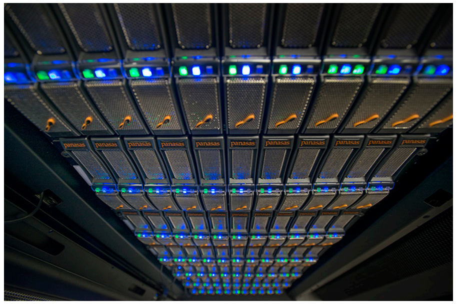
Context

- Centre for Environmental Data Analysis
  - A division of RAL Space
  - RAL Space is part of STFC
- CEDA is also part of NCAS and NCEO
- Government funded and research grants
  - EU H2020

- CEDA maintain a large archive of environmental data
  - Satellite data (esp. Sentinel and LandSat)
  - Climate and forecast data (CMIP5, ECMWF ERA-I, ERA-40)
  - Air measurement campaigns (EUFAR)
  - Ground based measurements
  - Approximately **7 PB**, including some data that is only on tape
- Provide access to the data to the scientific community and some commercial companies.

JASMIN





- A "super data-cluster”
  - a data-intensive computer
  - … and a datacentre
- Brings the compute to the data
  - and the data to the compute

- For users it provides high-performance computing with:
  - Access to the archive
  - Storage on disk (user workspace, currently **10 PB**) and tape
  - Batch computing
  - Virtualised computing
  - Cloud computing
- A joint collaboration between CEDA and **STFC SCD** (Scientific Computing Division)

JASMIN Phase 4

- JASMIN is currently undergoing a major upgrade
  - **38.5 PB** of storage is being added
    - Including **5 PB** of Object Storage
  - **11 PB** of POSIX storage will be retired by the end of 2018
- Currently the computing environments have direct POSIX access to the data on disk
- However, with the IaaS (Infrastructure-as-a-Service) cloud model this is undesirable and may not be possible
- Using storage with a (S3) HTTP API overcomes this problem and provides access to the Object Store
  - Also allows access to off-site storage (e.g. personal AWS)

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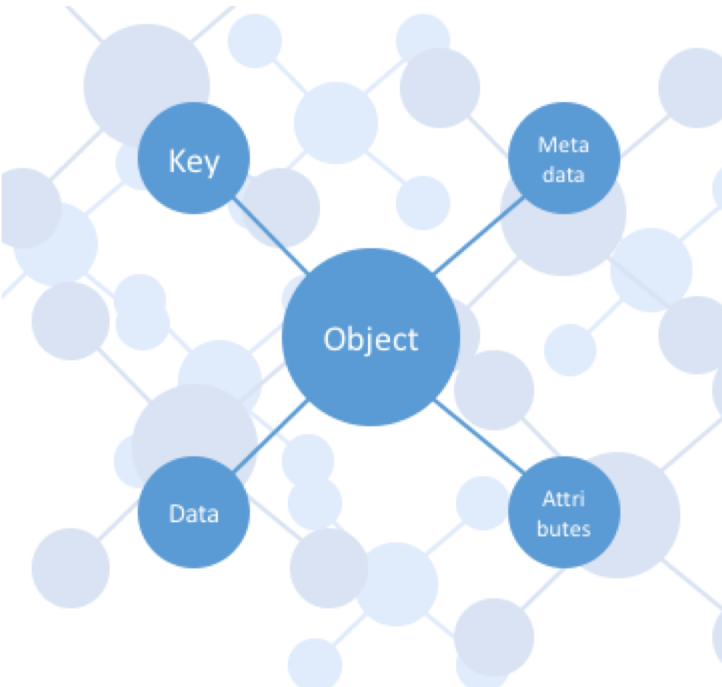
Object Storage

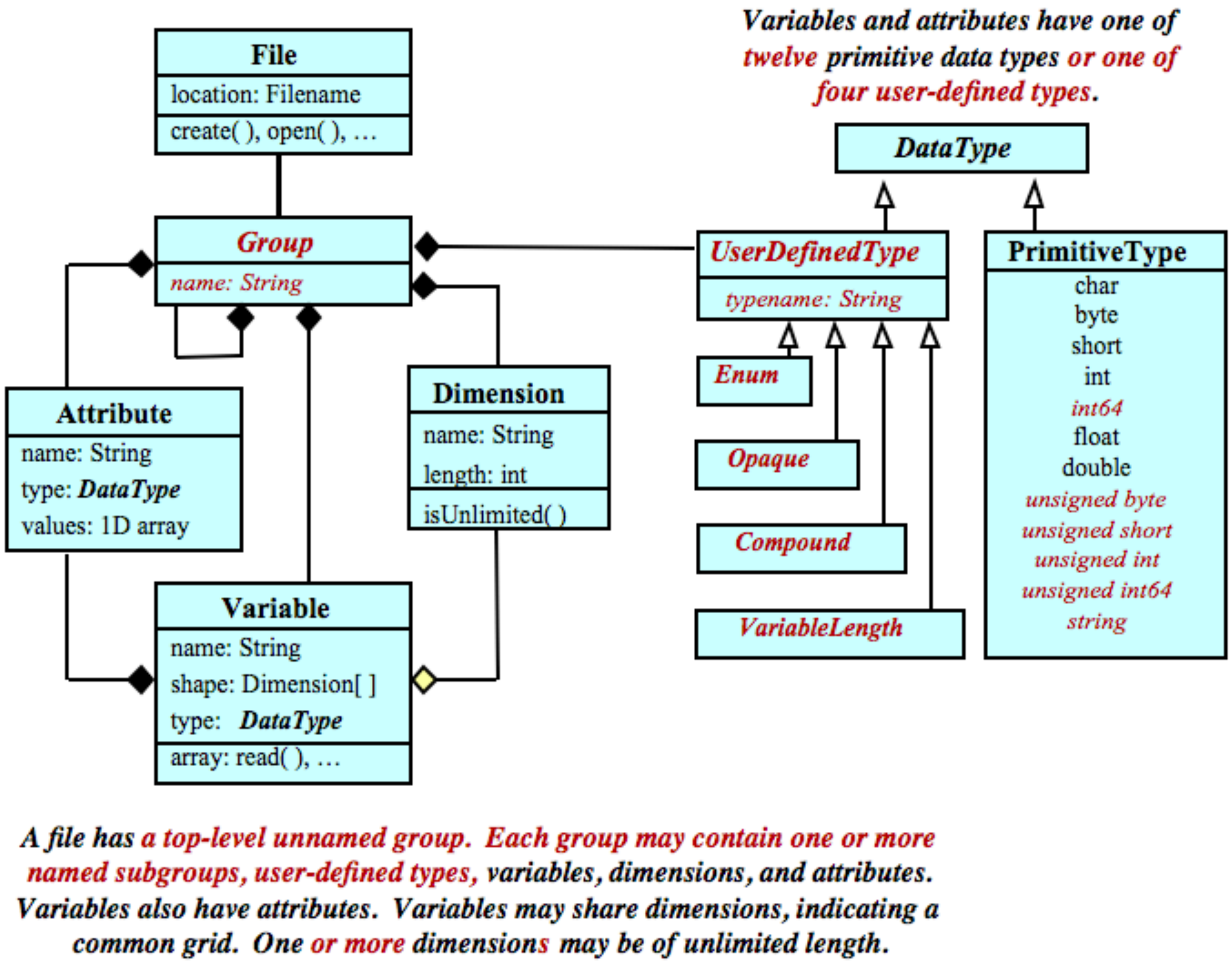


- A computer storage architecture in which *Objects* are stored in a flat structure
- Objects are identified by a unique key (a URL)
- Objects are organised into *Buckets*
- Object store can be accessed over a HTTP interface
  - Amazon's S3 HTTP REST API is the most popular
  - Data is uploaded and downloaded using PUT and GET operations respectively
- Supports two levels of metadata
  - System level metadata
  - Extendable metadata
- Allows searching for data without opening the file and custom searches for user data

What is a netCDF file?

- Network Common Data Form
- Array oriented data format
  - Multidimensional array variables
    - Variables are typed (int, float, etc.)
  - Coordinates for the dimensions (time, lat, lon, height, etc.)
  - Metadata for the variables (typed, including string)
  - Global metadata
  - Can take a “slice” (subdomain) from an array
- http://www.unidata.ucar.edu/software/netcdf/docs/user_guide.html

Structure of a netCDF file



http://www.unidata.ucar.edu/software/netcdf/docs/netcdf_data_set_components.html

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Structure of a netCDF file

The most useful command: **ncdump -h <filename>**

```
netcdf cru_ts3.24.01.1901.1910.tmp.dat {
dimensions:
     lon = 720 ;
     lat = 360 ;
     time = UNLIMITED ; // (120 currently)
variables:
     double lon(lon) ;
          lon:long_name = "longitude" ;
          lon:units = "degrees_east" ;
     double lat(lat) ;
          lat:long_name = "latitude" ;
          lat:units = "degrees_north" ;
     double time(time) ;
          time:long_name = "time" ;
          time:units = "days since 1900-1-1" ;
          time:calendar = "gregorian" ;
     double tmp(time, lat, lon) ;
          tmp:long_name = "near-surface temperature" ;
          tmp:units = "degrees Celsius" ;
          tmp:correlation_decay_distance = 1200. ;
          tmp:_FillValue = 9.96920996838687e+36 ;
          tmp:missing_value = 9.96920996838687e+36 ;
```

Dimension definitions

Dimension variables

Attributes

Field Variable

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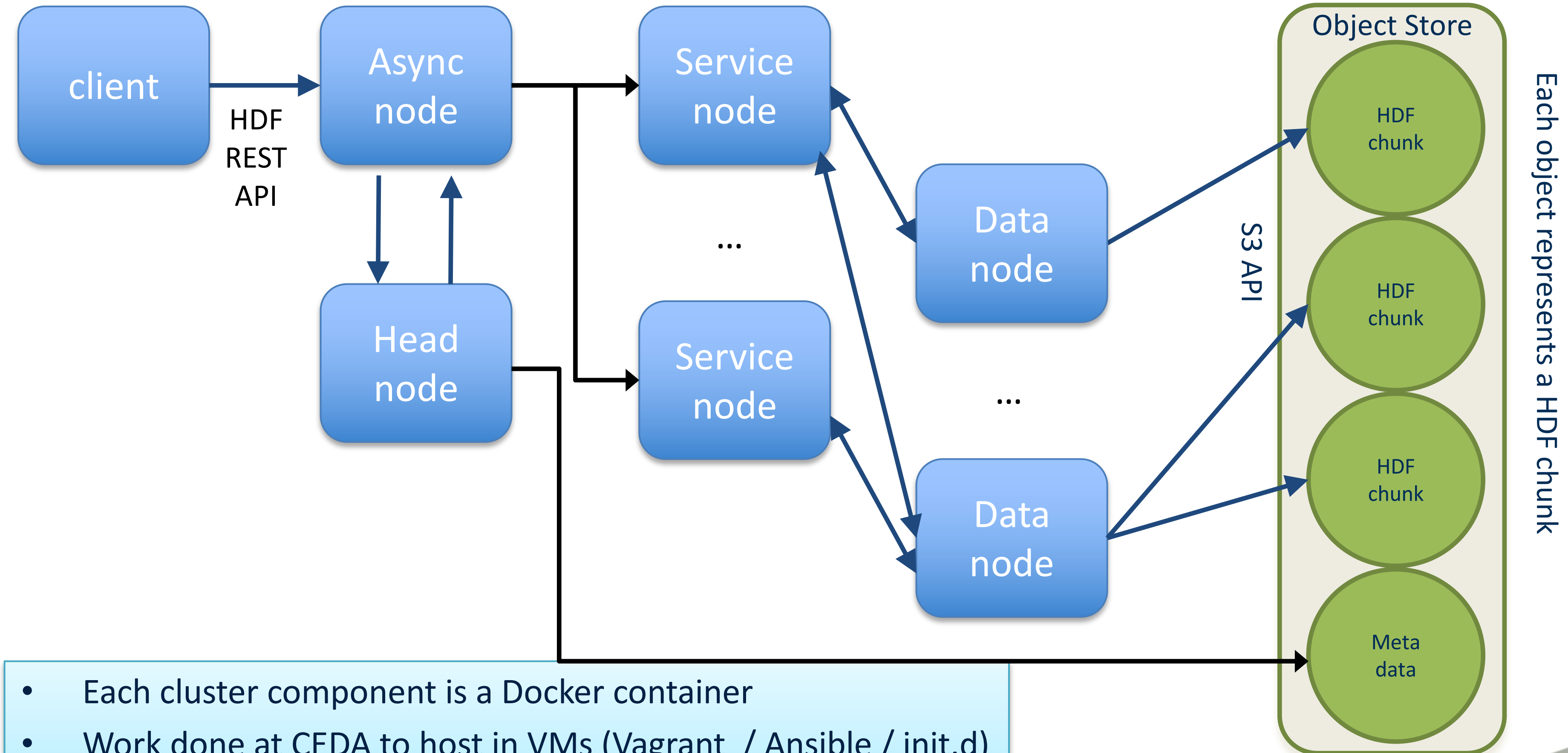
Writing netCDF files to object store

- It’s easy enough to write the whole file as an object, using minio API or boto3 API (Amazon’s API)
- Numerous disadvantages:
  1. Have to read / write the entire file at once to the object store
  2. Could use **range** function of (S3 API) but performance is unknown
  3. Does not permit parallel read / writes
  4. Have to read the entire file just to search the metadata!
- Instead we propose a method of splitting a netCDF file into fragments consisting of:
  1. A master array file, containing the variable definitions and metadata
  2. A number of subarray files containing subdomains of the variable data

HDF cloud and S3-netCDF

- **HDF cloud** from the HDF group also solves some of these problems
- HDF cloud has a cluster / server architecture:
  - The client connects to the cluster
  - The cluster serves the data from the object store to the client
  - The cluster load balances the requests
- **S3-netCDF** has a client-only model:
  - The client connects directly to the object store
  - The user is responsible for the load balancing
- We wanted to provide an easy to use library that can be used in the user workspaces for their own data

HSDS / HDF Cloud



- Each cluster component is a Docker container
- Work done at CEDA to host in VMs (Vagrant / Ansible / init.d)
- Client connects using h5pyd Python library (HDF REST API)

Key differences between HDF Cloud and S3netCDF4

HDF Cloud

- Any HDF file
- Connect using any HDF REST API client
- Cluster oriented architecture
- Parallel reads / writes limited to data nodes in the cluster
- Read / write fragments only to S3
- Fragments are HDF chunks with no semantic information

S3netCDF4

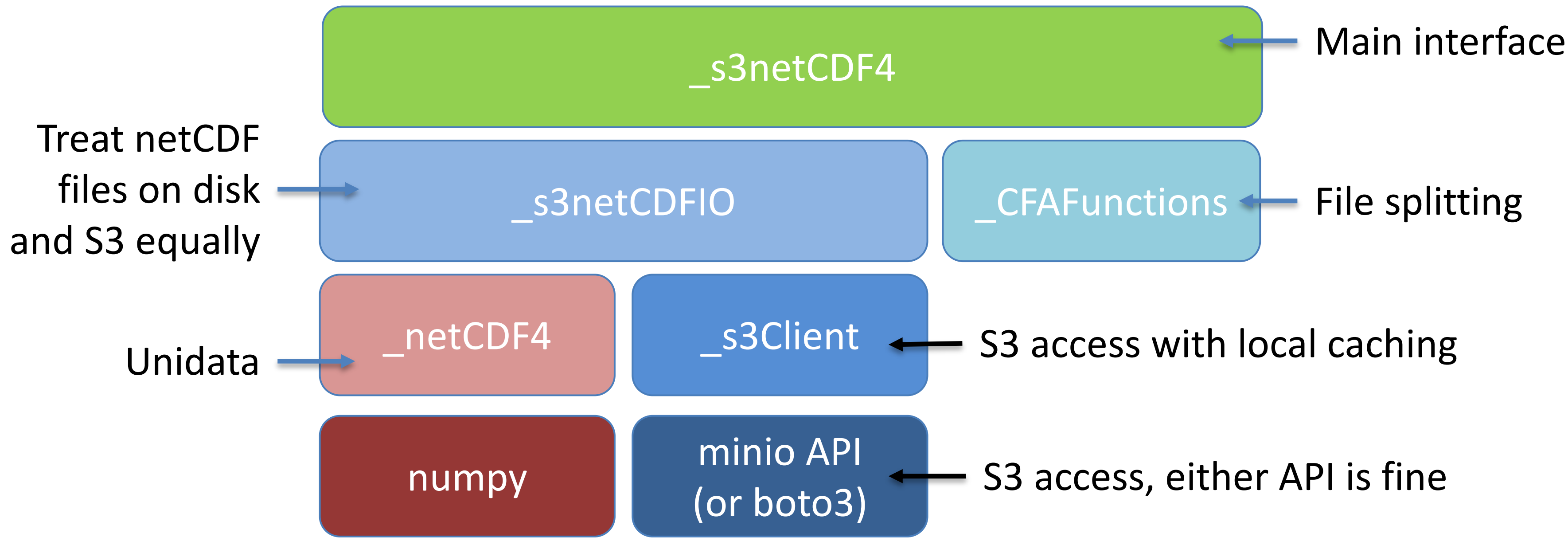
- netCDF4 & netCDF3 only
- Python only (currently)
- Client oriented architecture
- Parallel reads / writes limited to cores on the client machine
- Read / write fragments to S3, OpenDAP or local disk
- Fragments are self contained netCDF files
- Aggregation / data cube

S3-netCDF-python

- The library is implemented as a subclass of the standard Unidata python package (netCDF4.Dataset)

- Three main components:
  - **The interface** – matches netCDF4.Dataset as closely as possible
  - **A client** to read / write objects from / to a S3 object store, with the ability to stream to / from memory or to cache objects to disk, with sensible choices made based on available memory, object size and user input
  - **An array splitter** to split large netCDF4 variables into smaller ones, using the netCDF-CFA conventions

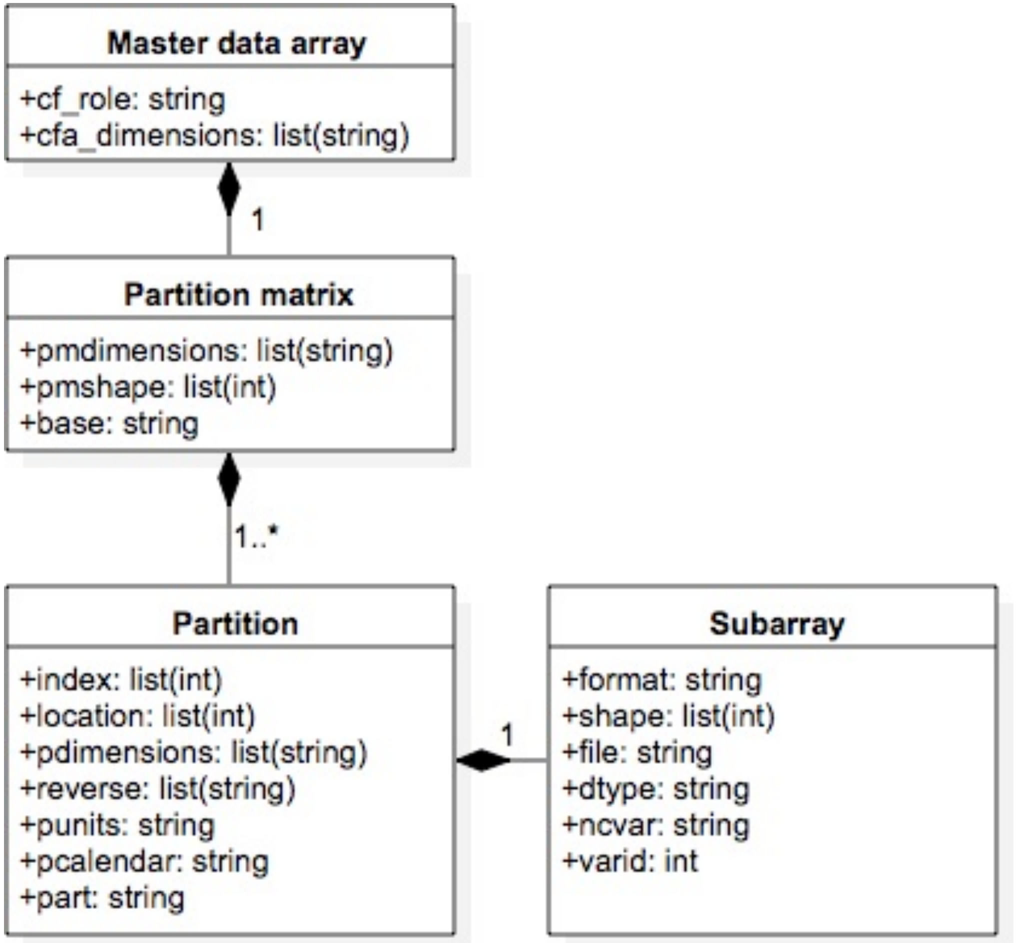
S3-netCDF software stack



CFA conventions

- Climate and forecast (CF) aggregation rules
  - Describe how multiple CF fields may be combined into one larger field
  - CFA-netCDF conventions for their efficient storage in netCDF files
  - Extension to netCDF via JSON encoded attributes
- A **master array** file (*kBs in size*)
  - Domains and metadata for a number of variables
  - Coordinates for the domains
  - Metadata for the subarrays, position in the master array
  - No field data
- A number of **subarray** files (*a single object, MBs to GBs in size*)
  - Subdomain and metadata (replicated from master array)
  - Coordinates for the subdomain
  - Field data

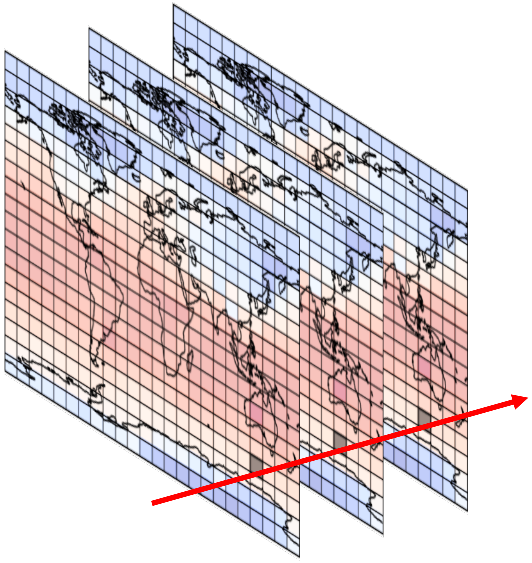
CFA Conventions

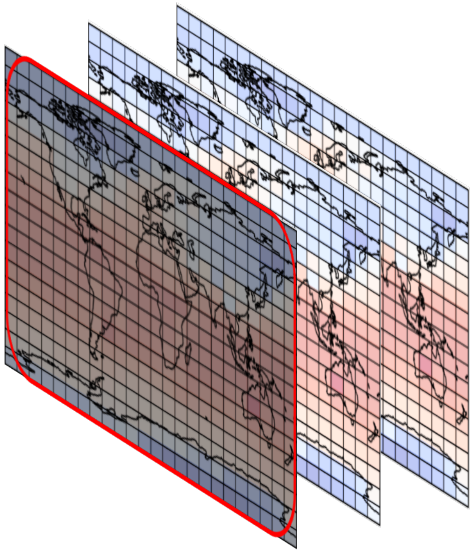


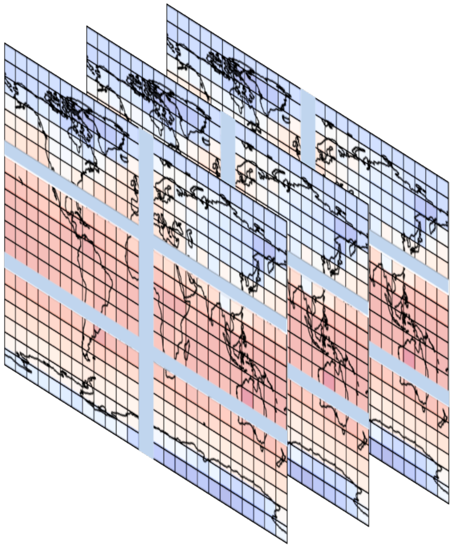
File splitting strategy

- NetCDF files are first split by **group**, then **variable**, then each variable is split into sub-domains. These sub-domains form the **sub-array** files.
- Access to the variable data involves reading and writing to the **sub-array** files.
- The size of the **sub-arrays** is optimised for two reading and writing use cases:
    1. The user reads a single spatial point (grid-box) for all the timesteps
    2. The user reads all the data (field) for a single timestep

File splitting strategy







1. $N = n_T/d_T$

2. $N = n_{lat}/d_{lat} * n_{lon}/d_{lon}$

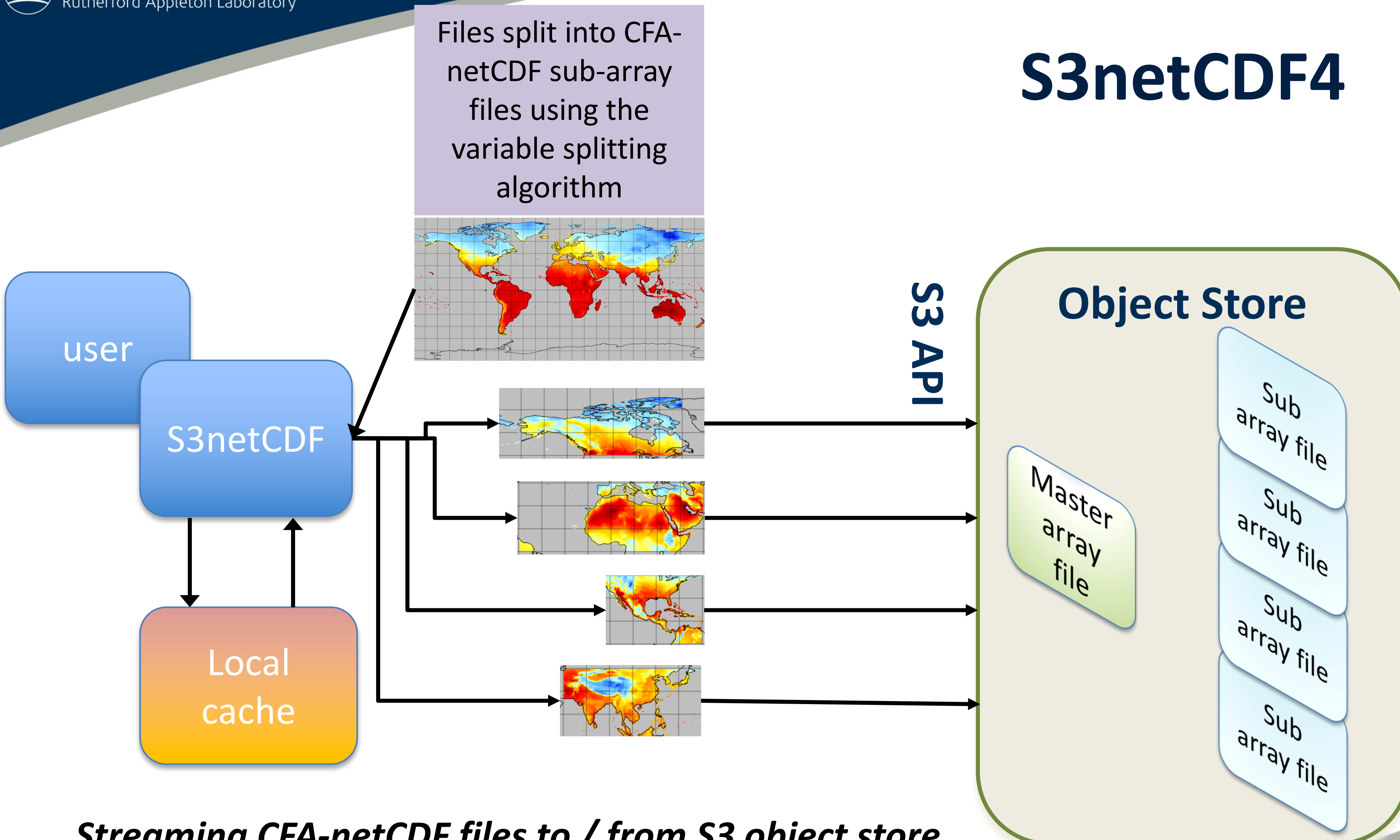
3. Approximately equal size "fragments"

N = number of operations needed to read entire timeseries / field
n = number of elements in the dimension
d = number of splits (divisions) in the dimension to form the sub-arrays

Reading / writing and data collection

- Client based architecture
  - A user library
  - Number of parallel reads limited to cores on client machine
  - Could be containerised (Docker) and multiple instances load-balanced (Kubernetes) for a server architecture
- Reading / writing consists of three stages:
  - Determine which subarrays are in the slice of the master array
  - Fetch the subarray data to either memory or a cached file
  - Copy the subarray data from memory to a memory mapped array

S3netCDF4



Streaming CFA-netCDF files to / from S3 object store

Why “semantic”?

- The master array file contains all the metadata and domains for all the subarrays
  - Only need to read the master array file to search the data
- Each subarray file contains all of its metadata and subdomain as well
  - Can reconstruct the master array file if it is lost
- The array splitter knows what each dimension represents (time, latitude, longitute, etc.) and acts accordingly
- Also good for aggregation
  - Add field data as it becomes available, e.g. each timestep of a GCM run
  - No need to rewrite the entire file – just the master array file and new subarray file

Current status and future work

- Current status:
  - Read / write to object store, disk or openDAP
  - Can take a slice, and only the subarray files in the slice are read from / written to
  - Mostly code compatible with netCDF4
  - Read and write subarray files in parallel (Python threads found to be the fastest)
- Future work:
  - SemSL – Semantic storage layers

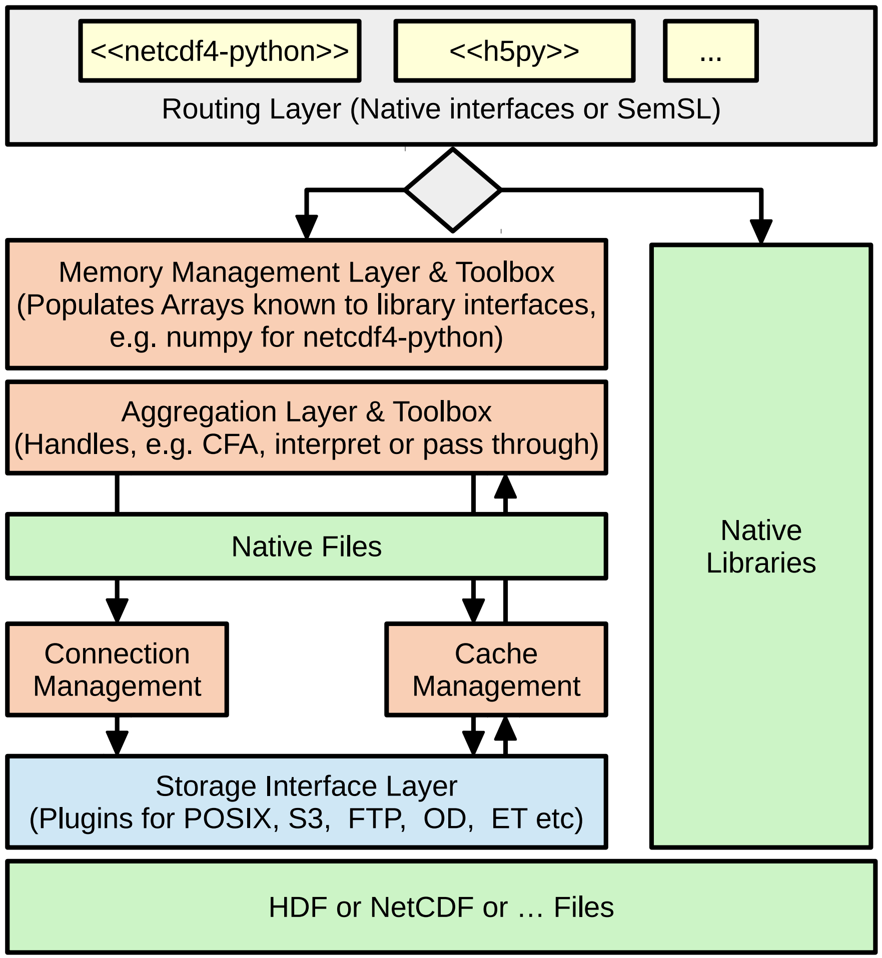
SemSL
Beyond object stores and netCDF

- ESiWACE project to expand on the capabilities of S3-netCDF
- Extend the fragmenting to other file formats:
  - netCDF *
  - HDF5 *
  - ESA SAFE
  - Tar files
  - Zip files
- Each of these “frontends” will be based upon existing libraries, e.g. netCDF4, h5py, etc.
  - Inherited and overloaded member functions where possible

SemSL
Beyond object stores and netCDF

- Extend the write capability to other storage technologies:
  - S3 / object store / AWS *
  - POSIX disk *
  - Parallel file systems
  - FTP *
  - Tape
- These "backends" will be based up existing libraries:
  - Boto3
  - FTPlib

SemSL – software architecture



SemSL

- The *Memory Managment* layer creates memory-mapped array objects, or memory-mapped file objects for non- array file-formats
- The *Aggregation Layer* handles the reading and writing of a *Master-File* and its *Fragments*
- *Cache Management:* A virtual or physical cache to temporarily stage files
- The *Connection Management* function allows connections to persist and be reused when reading / writing fragments
- The *Storage interface layer* provides a common interface to any number of external storage systems

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References

- S3-netCDF-python github
  https://github.com/cedadev/S3-netcdf-python
- Unidata netCDF4 package
  http://unidata.github.io/netcdf4-python/
- netCDF CFA conventions
  http://www.met.reading.ac.uk/~david/cfa/0.4/

Example code - write

```
# create a NETCDF4 file and upload to S3 storage
# this just follows the tutorial at http://unidata.github.io/netcdf4-python/
with Dataset(S3_WRITE_NETCDF_PATH, mode='w', diskless=True, format="CFA3") as s3_data:
    # create the dimensions
    leveld = s3_data.createDimension("level", len(levels_data))
    timed = s3_data.createDimension("time", None)
    latd = s3_data.createDimension("lat", 196)
    lond = s3_data.createDimension("lon", 256)
    # create the dimension variables
    times = s3_data.createVariable("time", "f8", ("time",))
    levels = s3_data.createVariable("level", "i4", ("level",))
    latitudes = s3_data.createVariable("lat", "f4", ("lat",))
    longitudes = s3_data.createVariable("lon", "f4", ("lon",))
    # create the field variable
    temp = s3_data.createVariable("tmp", "f4", ("time", "level", "lat", "lon"))

    # add some attributes
    s3_data.source = "netCDF4 python module tutorial"
    latitudes.units = "degrees north"
    longitudes.units = "degrees east"
    levels.units = "hPa"
    temp.units = "K"
    times.units = "hours since 0001-01-01 00:00:00.0"
    times.calendar = "gregorian"
```

Example code - read

```
# Test opening a CFA file on the object
with Dataset(WAH_S3_DATASET_PATH, 'r') as nc_file:
    nc_var = nc_file.getVariable("field8")
    print nc_var.shape
    print nc_var.dimensions
    print nc_var.name
    print nc_var.datatype
    print nc_var.size
    print type(nc_var)
    print np.mean(nc_var[0:10,0,40:80,40:80])

# load the original file and take the mean
with Dataset(WAH_NC4_DATASET_PATH) as src_file:
    src_var = src_file.variables["field8"]
    print type(src_var)
    print np.mean(src_var[0:10,0,40:80,40:80])
```