High-Perfomance Data Analytics in eScience

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esiwace
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Session outline

Introduction to Big Data, HPDA and data challenges in eScience

Introduction to the Ophidia HPDA Framework

Ophidia core concepts: architecture, storage model, operators and primitives, terminal and deployment

Analytics workflows with Ophidia

Ophidia Python bindings: PyOphidia

Practical PyOphidia tutorial

Climate analysis challenges & issues

Effective scientific analysis requires *novel solutions* able to cope with ***big data volumes***

Several key challenges and practical issues related to large-scale climate analysis

- Setup of a data analysis experiment requires the ***download of (multiple) input data***
  - *Data download is a big barrier for climate scientists*
  - *Reducing data movement is essential*
- The complexity of the analysis leads to the need for ***end-to-end workflow support***
  - *Data analysis* requires *highly-scalable solutions* able to *parallelize* the processing
  - Analysing large datasets involves *running tens/hundreds of analytics operators*
- Large data volumes pose ***strong requirements in terms of computational and storage resources***

High Performance Data Analytics for eScience

- *Computational science modeling and data analytics are both crucial in scientific research*
  - *Their coexistence in the same (current) software infrastructure is not trivial*
- *The convergence of the solutions and technology from the Big Data and HPC software ecosystems is a key factor for accelerating scientific discovery*

→ ***High-Performance Data Analytics (HPDA)***

- *New computing paradigms, data management approaches and job management solutions are being designed by the scientific software community*
- *Higher-level programming approaches* for data analytics are required to effectively exploit the resources and improve scientists' productivity

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Ophidia HPDA framework

Ophidia (http://ophidia.cmcc.it) is a CMCC Foundation research project addressing data challenges for eScience

- A **HPDA framework** for multi-dimensional scientific data joining HPC paradigms with scientific data analytics approaches
- **In-memory** and **server-side** data analysis exploiting parallel computing techniques
- Multi-dimensional, array-based, storage model and partitioning schema for scientific data leveraging the **datacube** abstraction
- End-to-end mechanisms to support **interactive analysis, complex experiments** and **large workflows** on scientific data

Ophidia

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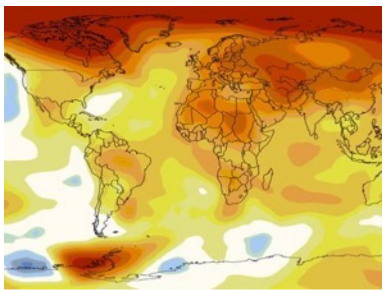
S. Fiore, D. Elia, C. Palazzo, F. Antonio, A. D'Anca, I. Foster, G. Aloisio, "Towards High Performance Data Analytics for Climate Change", ISC High Performance 2019, LNCS Springer, 2019

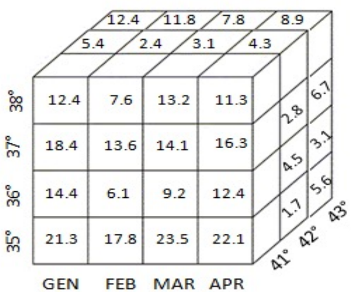
A paradigm shift

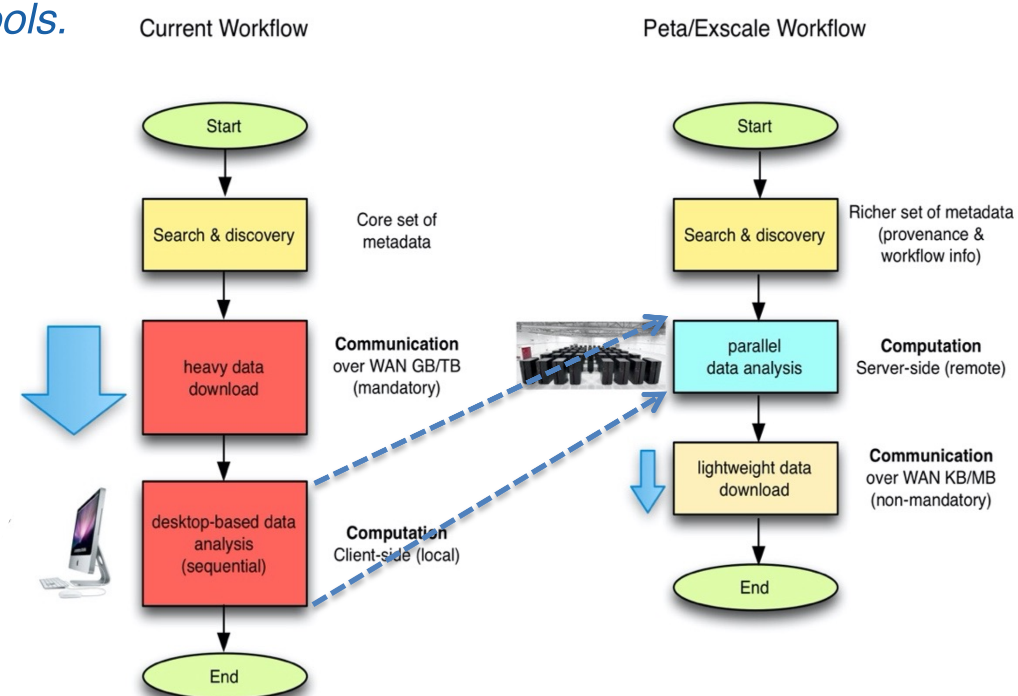
Volume, variety, velocity are key challenges for big data in general and for climate change science in particular. Client-side, sequential and disk-based workflows are three limiting factors for the current scientific data analysis tools.



Earth System Grid Federation

ESGF



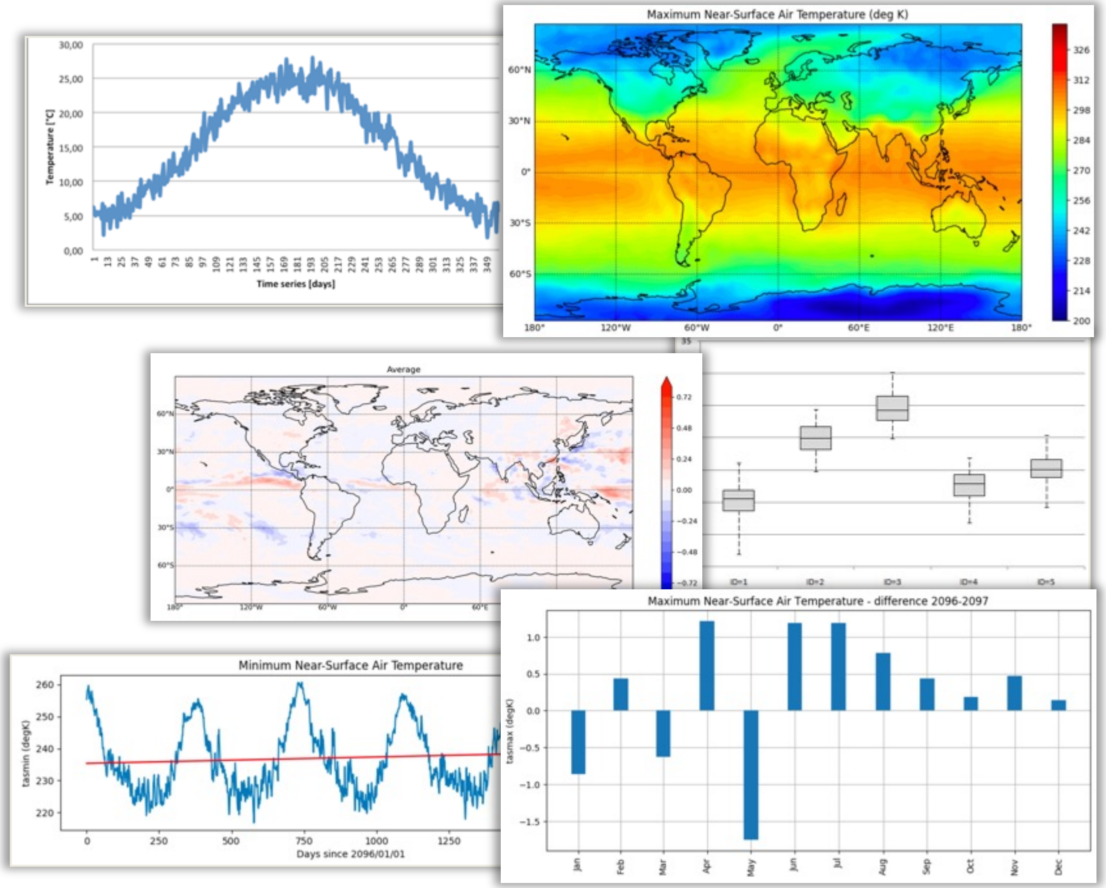


S. Fiore, A. D'Anca, C. Palazzo, I. Foster, D. N. Williams, G. Aloisio, "Ophidia: toward bigdata analytics for eScience", ICCS2013 Conference, Procedia Elsevier, 2013

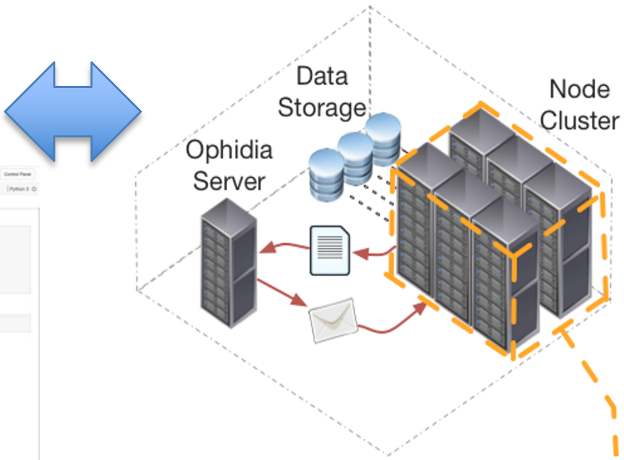
Data analytics requirements and use cases

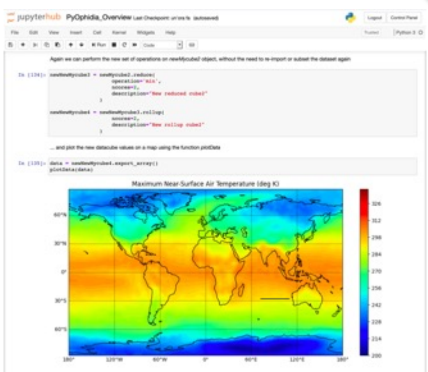
Requirements and needs focus on:

- *Time series analysis*
- *Data subsetting*
- *Model intercomparison*
- *Multi-model means*
- *Massive data reduction*
- *Data transformation*
- *Parameter sweep experiments*
- *Maps generation*
- *Ensemble analysis*
- *Data analytics workflow support*



Server-side paradigm and execution modes





Oph_Term: a terminal-like commands interpreter serving as a client for the Ophidia framework

PyOphidia: a Python interface for datacube management & analytics with Ophidia

Multiple execution modes:

- *Interactive data analysis*
- *Batch processing*
- *Python notebooks and applications*
- *Workflows of operators*

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Ophidia architecture: overview

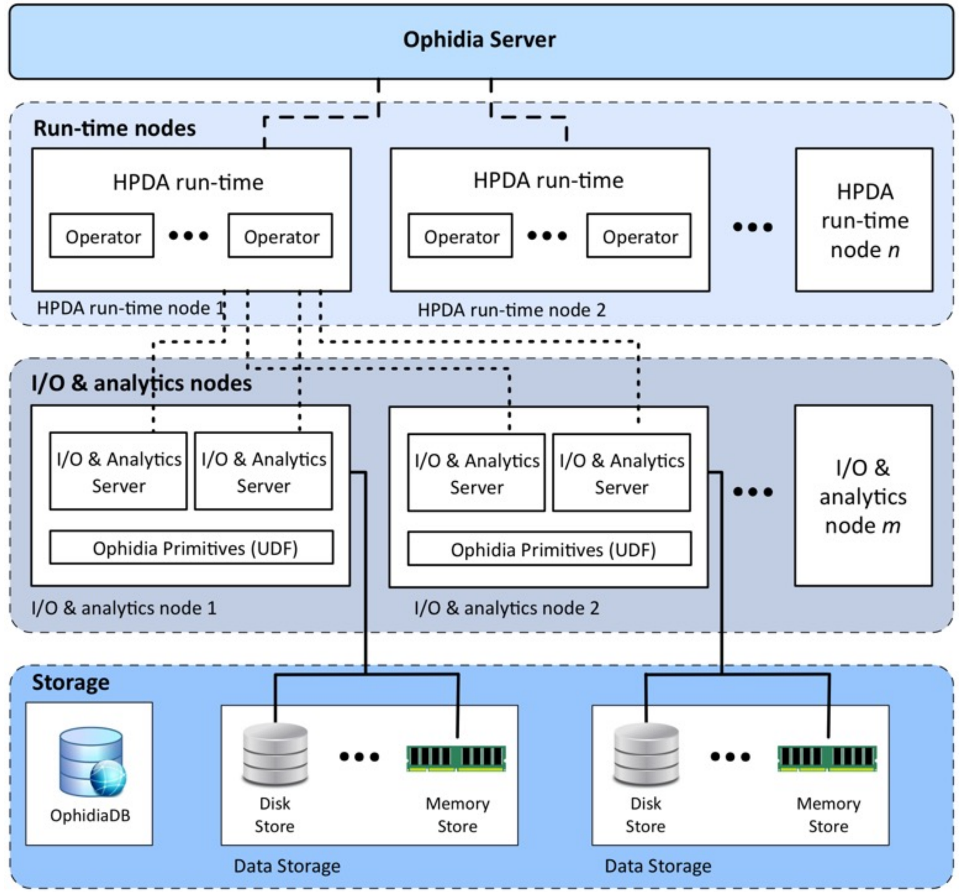
Front end

Runtime system

I/O & Analytics servers

Storage layer

System catalog



Ophidia architecture: storage layer & model

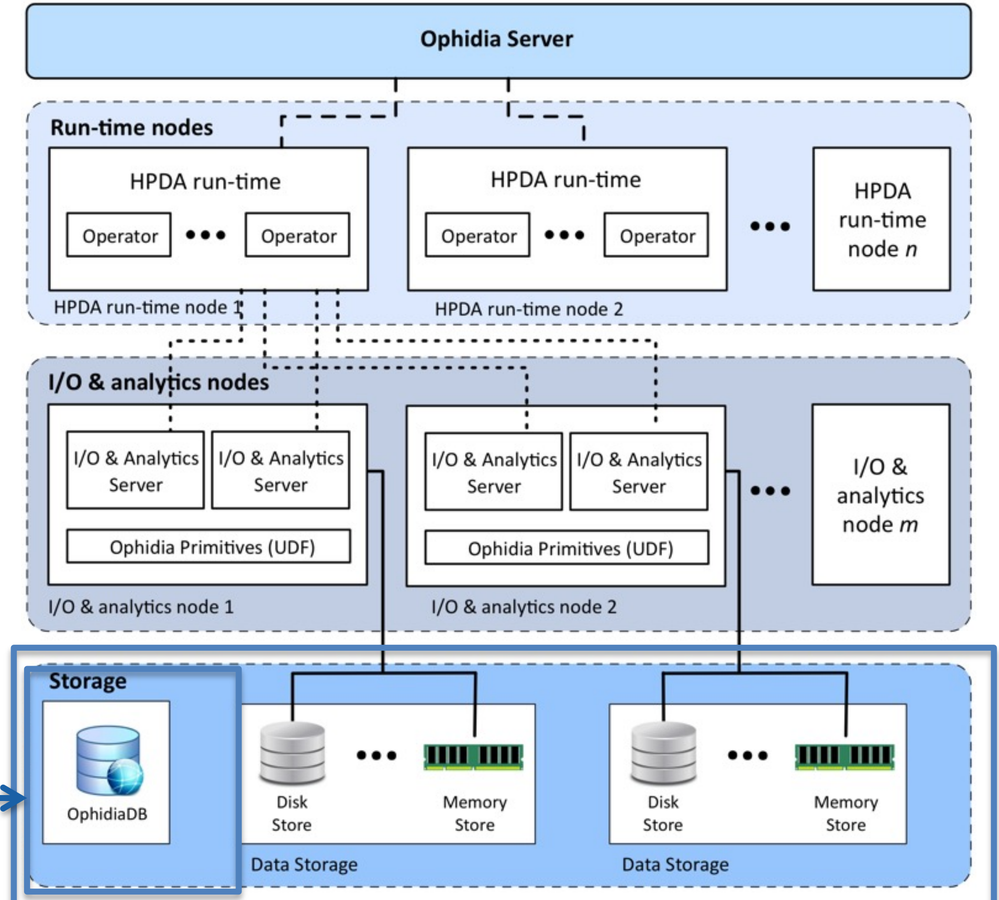
Distributed *hardware resources to manage storage*

Ophidia implements the ***datacube abstraction*** *from OLAP*

The storage model relies on ***implicit*** *(array-based) and* ***explicit*** *(tuple-based)* ***dimensions*** *for specific representations of data*

Data partitioned *in a hierarchical fashion over the storage according to the storage model & partitioning schema*

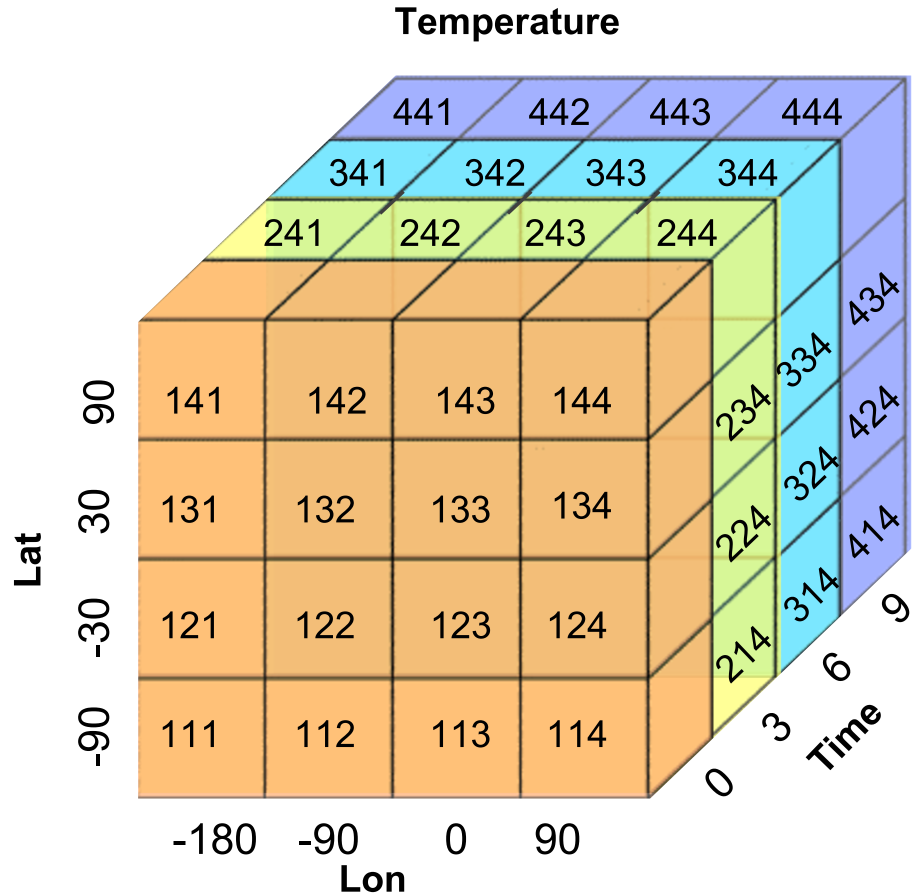
OphidiaDB is the system catalog: maps data fragmentation and tracks metadata



S. Fiore, D. Elia, C. Palazzo, F. Antonio, A. D'Anca, I. Foster, G. Aloisio, "Towards High Performance Data Analytics for Climate Change", ISC High Performance 2019, LNCS Springer, 2019

From NetCDF to datacube

```
netcdf test {
dimensions:
    lat = 4 ;
    lon = 4 ;
    time = UNLIMITED // (4 currently) ;
variables:
    double lon(lon) ;
    double lat(lat) ;
    double time(time) ;
    float Temperature(time, lat, lon) ;
data:
    lon = -180, -90, 0, 90 ;
    lat = -90, -30, 30, 90 ;
    time = 0, 3, 6, 9 ;
    temperature =
        111, 112, 113, 114,
          121, 122, 123, 124,
          131, 132, 133, 134,
          141, 142, 143, 144,
        211, 212, 213, 214,
          221, 222, 223, 224,
          231, 232, “33, 234,
          241, 242, 243, 244,
        ...
```



The datacube abstraction naturally fits for scientific multi-dimensional data, like climate data

From NetCDF to Ophidia

```
netcdf test {
dimensions:
    lat = 4 ;
    lon = 4 ;
    time = UNLIMITED // (4 currently) ;
variables:
    double lon(lon) ;
    double lat(lat) ;
    double time(time) ;
    float Temperature(time, lat, lon) ;
data:
    lon = -180, -90, 0, 90 ;
    lat = -90, -30, 30, 90 ;
    time = 0, 3, 6, 9 ;
    temperature =
        111, 112, 113, 114,
          121, 122, 123, 124,
          131, 132, 133, 134,
          141, 142, 143, 144,
        211, 212, 213, 214,
          221, 222, 223, 224,
          231, 232, 233, 234,
          241, 242, 243, 244,
        311, 312, 313, 314,
          ...
```

Defined as:
implicit dimension

NetCDF

		Temperature			
lat	lon	time[0]	time[1]	time[2]	time[3]
-90	-180	111	211	311	411
-90	-90	112	212	312	412
-90	0	113	213	313	413
-90	90	114	214	314	414
-30	-180	121	221	321	421
-30	-90	122	222	322	422
-30	0	123	223	323	423
-30	90	124	224	324	424
30	-180	131	231	331	431
30	-90	132	232	332	432
30	0	133	233	333	433
30	90	134	234	334	434
90	-180	141	241	341	441
90	-90	142	242	342	442
90	0	143	243	343	443
90	90	144	244	344	444

Ophidia

From NetCDF to Ophidia

```
netcdf test {
dimensions:
    lat = 4 ;
    lon = 4 ;
    time = UNLIMITED // (4 currently) ;
variables:
    double lon(lon) ;
    double lat(lat) ;
    double time(time) ;
    float Temperature(time, lat, lon) ;
data:
    lon = -180, -90, 0, 90 ;
    lat = -90, -30, 30, 90 ;
    time = 0, 3, 6, 9 ;
    temperature =
        111, 112, 113, 114,
          121, 122, 123, 124,
          131, 132, 133, 134,
          141, 142, 143, 144,
        211, 212, 213, 214,
          221, 222, 223, 224,
          231, 232, 233, 234,
          241, 242, 243, 244,
        311, 312, 313, 314,
          ...
```

NetCDF

Defined as:
explicit dimensions

		Temperature			
lat	lon	time[0]	time[1]	time[2]	time[3]
-90	-180	111	211	311	411
-90	-90	112	212	312	412
-90	0	113	213	313	413
-90	90	114	214	314	414
-30	-180	121	221	321	421
-30	-90	122	222	322	422
-30	0	123	223	323	423
-30	90	124	224	324	424
30	-180	131	231	331	431
30	-90	132	232	332	432
30	0	133	233	333	433
30	90	134	234	334	434
90	-180	141	241	341	441
90	-90	142	242	342	442
90	0	143	243	343	443
90	90	144	244	344	444

Ophidia

From NetCDF to Ophidia

```
netcdf test {
dimensions:
    lat = 4 ;
    lon = 4 ;
    time = UNLIMITED // (4 currently) ;
variables:
    double lon(lon) ;
    double lat(lat) ;
    double time(time) ;
    float Temperature(time, lat, lon) ;
data:
    lon = -180, -90, 0, 90 ;
    lat = -90, -30, 30, 90 ;
    time = 0, 3, 6, 9 ;
    temperature =
        111, 112, 113, 114,
          121, 122, 123, 124,
          131, 132, 133, 134,
          141, 142, 143, 144,
        211, 212, 213, 214,
          221, 222, 223, 224,
          231, 232, 233, 234,
          241, 242, 243, 244,
        311, 312, 313, 314,
          ...
```

NetCDF

Mapped to a single unique key

ID	Array			
1	111	211	311	411
2	112	212	312	412
3	113	213	313	413
4	114	214	314	414
5	121	221	321	421
6	122	222	322	422
7	123	223	323	423
8	124	224	324	424
9	131	231	331	431
10	132	232	332	432
11	133	233	333	433
12	134	234	334	434
13	141	241	341	441
14	142	242	342	442
15	143	243	343	443
16	144	244	344	444

Ophidia

From NetCDF to Ophidia

```
netcdf test {
dimensions:
    lat = 4 ;
    lon = 4 ;
    time = UNLIMITED // (4 currently) ;
variables:
    double lon(lon) ;
    double lat(lat) ;
    double time(time) ;
    float Temperature(time, lat, lon) ;
data:
    lon = -180, -90, 0, 90 ;
    lat = -90, -30, 30, 90 ;
    time = 0, 3, 6, 9 ;
    temperature =
        111, 112, 113, 114,
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          131, 132, 133, 134,
          141, 142, 143, 144,
        211, 212, 213, 214,
          221, 222, 223, 224,
          231, 232, 233, 234,
          241, 242, 243, 244,
        311, 312, 313, 314,
          ...
```
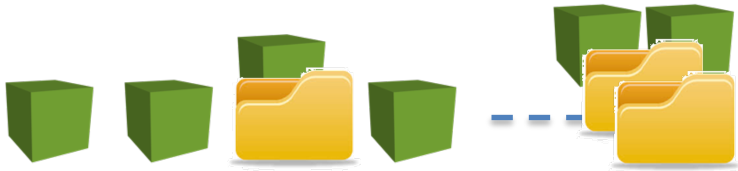

NetCDF

This long table is then horizontally partitioned in multiple fragments

		Temperature			
lat	lon	time[0]	time[1]	time[2]	time[3]
-90	-180	111	211	311	411
-90	-90	112	212	312	412
-90	0	113	213	313	413
-90	90	114	214	314	414
-30	-180	121	221	321	421
-30	-90	122	222	322	422
-30	0	123	223	323	423
		124	224	324	424
		131	231	331	431
		132	232	332	432
		133	233	333	433
30	90	134	234	334	434
90	-180	141	241	341	441
90	-90	142	242	342	442
90	0	143	243	343	443
90	90	144	244	344	444

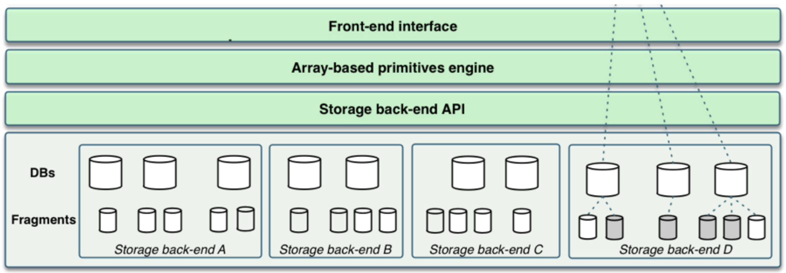
Ophidia

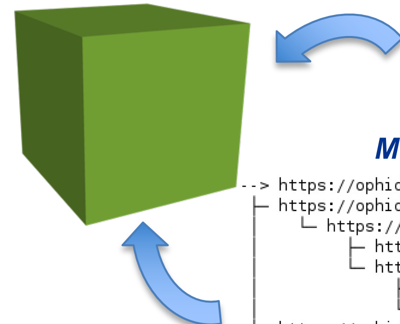
Data abstraction: cube space perspective



User perspective (datacube abstraction)

System perspective (internal storage representation)





System metadata of the datacube (size, distribution, etc.)

Metadata provenance

```
--> https://ophidia.cmcc.it:8443/162/169 (ROOT)
 ├ https://ophidia.cmcc.it:8443/162/170 (oph_reduce)
 │   └ https://ophidia.cmcc.it:8443/162/171 (oph_merge)
 │       ├ https://ophidia.cmcc.it:8443/162/172 (oph_aggregate2)
 │       └ https://ophidia.cmcc.it:8443/162/173 (oph_rollup)
 │           ├ https://ophidia.cmcc.it:8443/162/174 (oph_reduce)
 │           └ https://ophidia.cmcc.it:8443/162/175 (oph_reduce)
 ├ https://ophidia.cmcc.it:8443/162/176 (oph_aggregate)
 └ https://ophidia.cmcc.it:8443/162/177 (oph_aggregate)
```

CMD	BEHAVIOR
cd	change directory
mkdir	create a new folder
rm	remove an empty folder or hide (logically delete) a container
ls	list subfolders and containers in a folder
mv	move/rename a folder or a container

Metadata associated to the datacubes

Searching results

Id	Variable	Key	Type	Value
73693068	tas	standard_name	text	air_temperature
73693069	tas	long_name	text	Air Temperature
73693070	tas	comment	text	This is sampled synoptically.
73693071	tas	units	text	K
73693072	tas	original_name	text	temp2

S. Fiore, D. Elia, C. Palazzo, F. Antonio, A. D'Anca, I. Foster, G. Aloisio, "Towards High Performance Data Analytics for Climate Change", ISC High Performance 2019, LNCS Springer, 2019

Ophidia architecture: I/O & Analytics layer

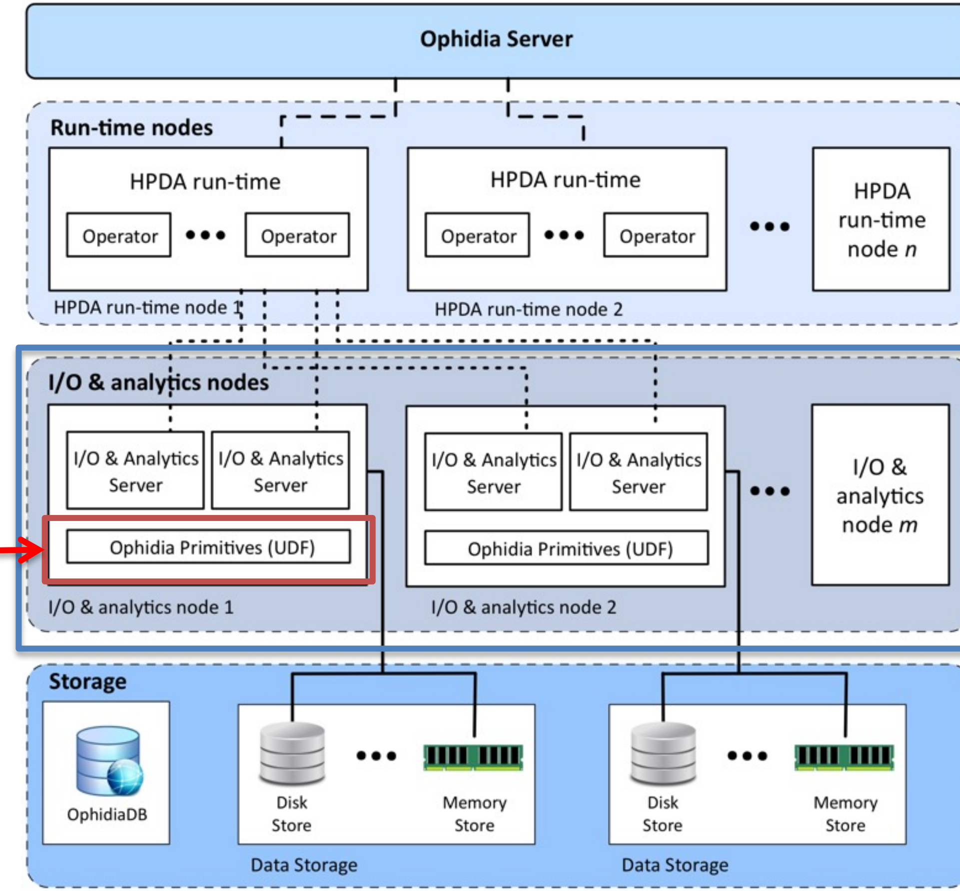
*Multiple **I/O & analytics nodes** execute one or more servers*

Servers can transparently interface to different storage back-ends

*Native **in-memory** analytics & I/O **engine** for **n-dimensional arrays***

*Servers run the (binary) array-based **Ophidia primitives** (UDF)*

Handles also I/O with NetCDF files, access and management of datacubes



D. Elia, S. Fiore, A. D'Anca, C. Palazzo, I. Foster, D. N. Williams, G. Aloisio (2016). "An in-memory based framework for scientific data analytics". In Proc. of the ACM Int. Conference on Computing Frontiers (CF '16), pp. 424-429.

Ophidia array-based primitives

Ophidia provides a **wide set of array-based primitives** (around 100) to perform:

- data summarization, sub-setting, predicates evaluation, statistical analysis, array concatenation, algebraic expression, regression, etc.

Primitives come as plugins (UDF) and are applied on a single datacube chunk (fragment)

Primitives can be nested to get more complex functionalities

New primitives can be easily integrated as additional plugins

oph_apply operator to run any primitive on a datacube

*oph_apply(oph_predicate(measure,'**x-298.15**','**>0**','**1**','**0**'))*

Ophidia Primitives documentation: http://ophidia.cmcc.it/documentation/users/primitives/index.html

Array-based primitives: nesting support

oph_boxplot(oph_subarray(oph_uncompress(measure), 1,18))

Single chunk or fragment (input)

INPUT TABLE 5 tuples x 50 elements

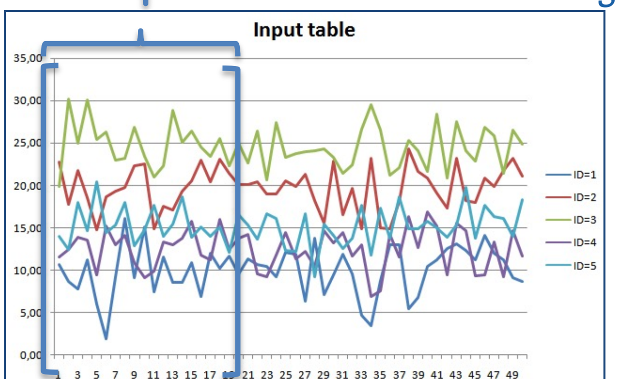
ID	MEASURE									
1	10,73	8,66	7,83	11,20	6,02	1,95	...	16,11	...	8,70
2	22,85	17,84	21,82	18,57	14,81	18,71	...	19,83	...	21,13
3	19,89	30,17	24,95	30,07	25,40	26,31	...	23,18	...	24,82
4	11,60	12,49	13,91	13,53	9,48	15,27	...	14,17	...	11,66
5	13,94	12,43	17,95	14,70	20,41	14,46	...	18,00	...	18,30

subarray(measure, 1,18)

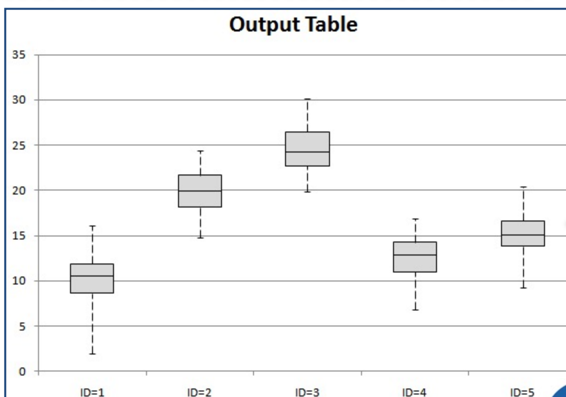
Single chunk or fragment (output)

OUTPUT TABLE 5 tuples x 5 elements (summary)

ID	MEASURE				
1	1,95	8,64	10,47	11,87	16,11
2	14,81	18,14	19,93	21,66	24,35
3	19,89	22,74	24,24	26,45	30,17
4	6,87	10,99	12,85	14,28	16,93
5	9,23	13,87	15,05	16,61	20,41



Scientific representation



Ophidia architecture: HPDA runtime layer

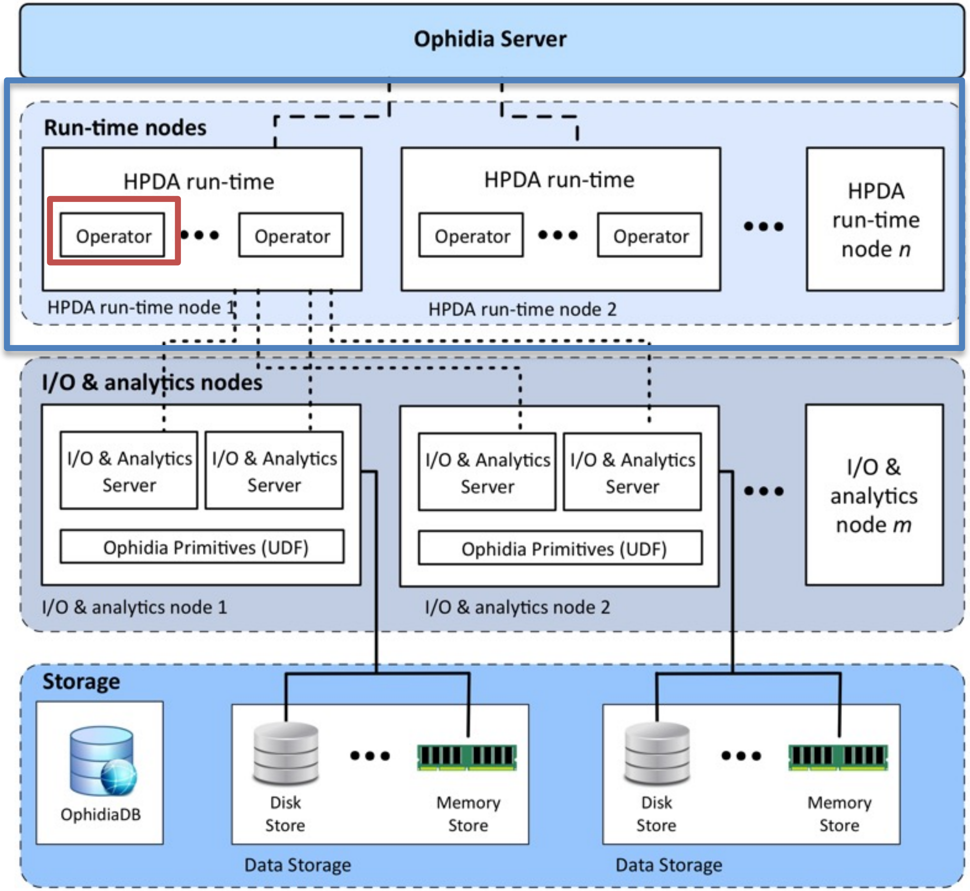
*The Ophidia HPDA runtime system can be executed with **multiple processes/threads** and **distributed over multiple nodes***

*Runtime defines a **multi-level parallel execution model:***

- *Datacube-level (HTC-based)*
- *Fragment-level (HPC-based: MPI+X)*

*Provides the environment for the execution of **parallel** MPI/Pthread-based **operators***

*Operators interact with the I/O & analytics servers to manipulate the entire set of fragments associated to a **whole datacube***



D. Elia, S. Fiore and G. Aloisio, "Towards HPC and Big Data Analytics Convergence: Design and Experimental Evaluation of a HPDA Framework for eScience at Scale," in IEEE Access, vol. 9, pp. 73307-73326, 2021

Ophidia operators

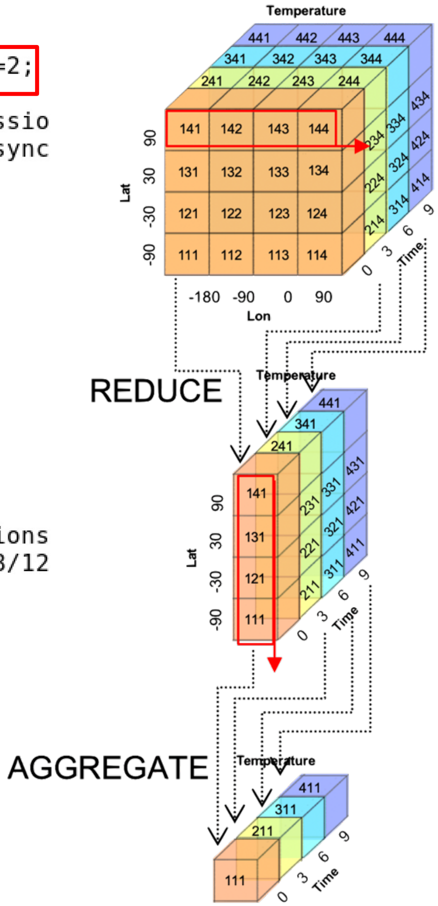
CLASS	PROCESSING TYPE	OPERATOR(S)
I/O	Parallel	OPH_IMPORTNC, OPH_EXPORTNC, OPH_CONCATNC, OPH_RANDUCUBE
Time series processing	Parallel	OPH_APPLY
Datacube reduction	Parallel	OPH_REDUCE, OPH_REDUCE2, OPH_AGGREGATE
Datacube subsetting	Parallel	OPH_SUBSET
Datacube combination	Parallel	OPH_INTERCUBE, OPH_MERGECUBES
Datacube structure manipulation	Parallel	OPH_SPLIT, OPH_MERGE, OPH_ROLLUP, OPH_DRILLDOWN, OPH_PERMUTE
Datacube/file system management	Sequential	OPH_DELETE, OPH_FOLDER, OPH_FS
Metadata management	Sequential	OPH_METADATA, OPH_CUBEIO, OPH_CUBESCHEMA
Datacube exploration	Sequential	OPH_EXPLORECUBE, OPH_EXPLORENC

About 50 operators for data and metadata processing

Ophidia operators documentation: http://ophidia.cmcc.it/documentation/users/operators/index.html

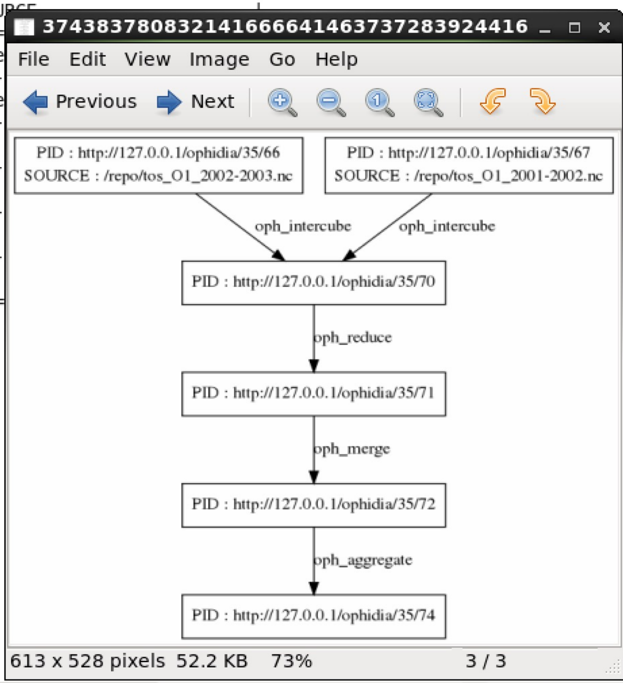
“data” operators

```
[12..3289] >> oph_reduce cube=http://127.0.0.1/ophidia/418/12717;operation=avg;ncores=2;nthreads=2;
[Request]:
operator=oph_reduce;cube=http://127.0.0.1/ophidia/418/12717;operation=avg;ncores=2;nthreads=2;sessio
nid=http://127.0.0.1/ophidia/sessions/127028404128222463341617004437753289/experiment;exec_mode=sync
;cwd=/;cdd=/;host_partition=auto;

[JobID]:
http://127.0.0.1/ophidia/sessions/127028404128222463341617004437753289/experiment?239#582

[Response]:
Output Cube
-----------
http://127.0.0.1/ophidia/418/12722

Execution time: 0.35 seconds
[12..3289] >> oph_aggregate operation=avg;ncores=2;nthreads=2;
[Request]:
operator=oph_aggregate;operation=avg;ncores=2;nthreads=2;sessionid=http://127.0.0.1/ophidia/sessions
/127028404128222463341617004437753289/experiment;exec_mode=sync;cube=http://127.0.0.1/ophidia/418/12
722;cwd=/;cdd=/;host_partition=auto;

[JobID]:
http://127.0.0.1/ophidia/sessions/127028404128222463341617004437753289/experiment?240#584

[Response]:
Output Cube
-----------
http://127.0.0.1/ophidia/418/12723

Execution time: 0.17 seconds
```



“metadata” operators

```
[37..4416] >> oph_cubeio
[Request]:
operator=oph_cubeio;sessionid=http://127.0.0.1/ophidia/sessions/374383780832141666641463737283924416/experiment;exec_mode=sync;ncores=1;cube=http://127.0.0.1/ophidia/35/74;cwd=/
;

[JobID]:
http://127.0.0.1/ophidia/sessions/374383780832141666641463737283924416/experiment?82#176

[Response]:
Cube Provenance
---------------

+=================================================================+===============+================================+========================+
| INPUT CUBE                                                      | OPERATION     | OUTPUT CUBE                    | SOURCE
+=================================================================+===============+================================+========================+
|                                                                 | ROOT          | http://127.0.0.1/ophidia/35/66 | /re
|-----------------------------------------------------------------|---------------|--------------------------------|----
|                                                                 | ROOT          | http://127.0.0.1/ophidia/35/67 | /re
|-----------------------------------------------------------------|---------------|--------------------------------|----
| http://127.0.0.1/ophidia/35/66 - http://127.0.0.1/ophidia/35/67 | oph_intercube | http://127.0.0.1/ophidia/35/70 |
|-----------------------------------------------------------------|---------------|--------------------------------|----
| http://127.0.0.1/ophidia/35/70                                  | oph_reduce    | http://127.0.0.1/ophidia/35/71 |
|-----------------------------------------------------------------|---------------|--------------------------------|----
| http://127.0.0.1/ophidia/35/71                                  | oph_merge     | http://127.0.0.1/ophidia/35/72 |
|-----------------------------------------------------------------|---------------|--------------------------------|----
| http://127.0.0.1/ophidia/35/72                                  | oph_aggregate | http://127.0.0.1/ophidia/35/74 |
+=================================================================+===============+================================+====

Cube Provenance Graph
---------------------

Directed Graph DOT string :
digraph DG {
        node    [shape=box]

        0       [label="PID : http://127.0.0.1/ophidia/35/74\n"]
        1       [label="PID : http://127.0.0.1/ophidia/35/72\n"]
        2       [label="PID : http://127.0.0.1/ophidia/35/71\n"]
        3       [label="PID : http://127.0.0.1/ophidia/35/70\n"]
        4       [label="PID : http://127.0.0.1/ophidia/35/66\nSOURCE : /repo/tos_O1_2002-2003.nc\n"]
        5       [label="PID : http://127.0.0.1/ophidia/35/67\nSOURCE : /repo/tos_O1_2001-2002.nc\n"]

        1->0    [label="oph_aggregate"]
        2->1    [label="oph_merge"]
```



Ophidia architecture: front-end layer

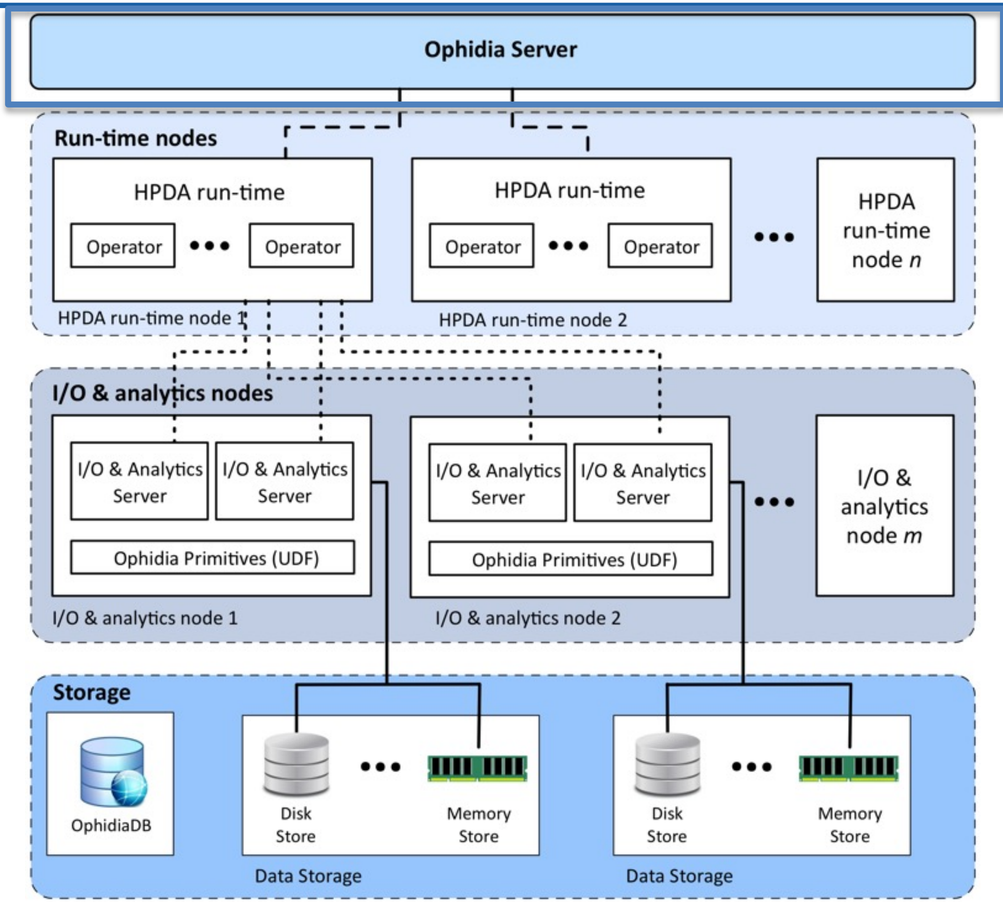
*The **Ophidia Server** is the **multi-interface** server front-end*

*Manages user **authN/authZ, sessions** and enables server-side computation*

*Handles **single task** and **workflows** execution and monitors their execution*

Remote interactions with:

- *the Ophidia terminal CLI*
- *PyOphidia Python API*
- *WPS clients*



C. Palazzo, A. Mariello, S. Fiore, A. D'Anca, D. Elia, D. N. Williams, G. Aloisio, "A Workflow-Enabled Big Data Analytics Software Stack for eScience", HPCS 2015, pp. 545-552

Ophidia Terminal

The **Ophidia Terminal**, a CLI bash-like client for the Ophidia HPDA Framework:

- Executing *interactive* data analytics sessions;
- Submit *batch* data analytics tasks of *workflows*;
- Experiment and operators *debugging*;
- *File system exploration* and *environment management*.

```
[11..4495] >> oph_list level=2;
[Request]:
operator=oph_list;path=;level=2;sessionid=http://127.0.0.1/ophidia/sessions/1112
38695229505952271558621818154495/experiment;exec_mode=sync;cdd=/;

[JobID]:
http://127.0.0.1/ophidia/sessions/111238695229505952271558621818154495/experiment?2#45

[Response]:
Ophidia Filesystem: /
---------------------

+===+====================+============================================+=============+
| T | PATH               | DATACUBE PID                               | DESCRIPTION |
+===+====================+============================================+=============+
| f | testFolder/        |                                            |             |
|---|--------------------|--------------------------------------------|-------------|
| c | test               | http://127.0.0.1/ophidia/2917/374976       |             |
+===+====================+============================================+=============+
```

On-demand deployment on HPC infrastructures

Target environment: *HPC cluster*

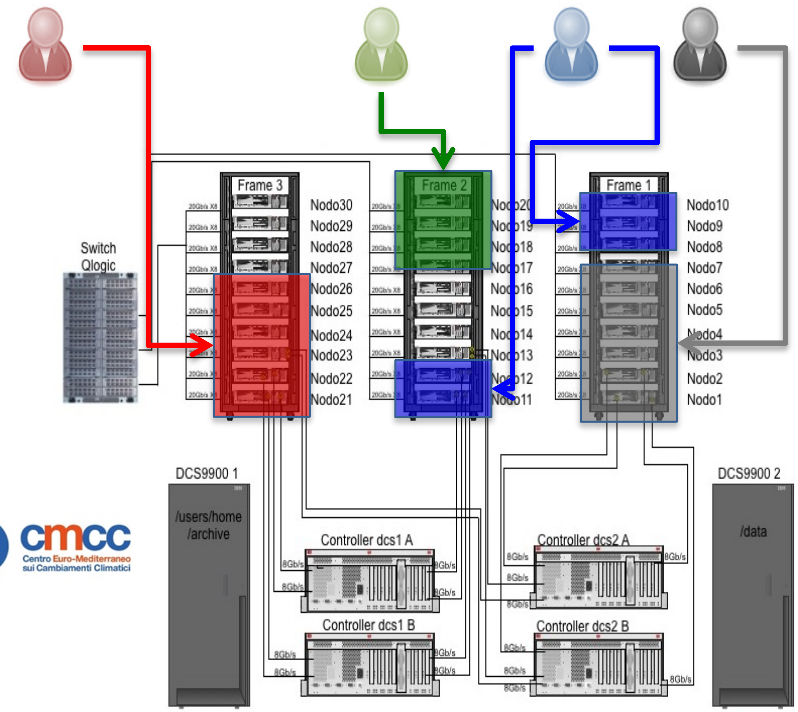
On-demand deployment of I/O & analytics servers

- `oph_cluster action=deploy;nhost=64;cluster_name=new;`
- `oph_cluster action=undeploy;cluster_name=new;`

Transparent interaction with scheduling systems

Zeus SuperComputer at CMCC: 1.2 PetaFlops, 348 nodes

Multiple isolated instances can be deployed simultaneously by different teams/users



Session outline

Introduction to Big Data, HPDA and data challenges in eScience

Introduction to the Ophidia HPDA Framework

Ophidia core concepts: architecture, storage model, operators and primitives, terminal and deployment

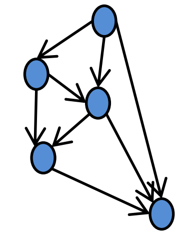
Analytics workflows with Ophidia

Ophidia Python bindings: PyOphidia

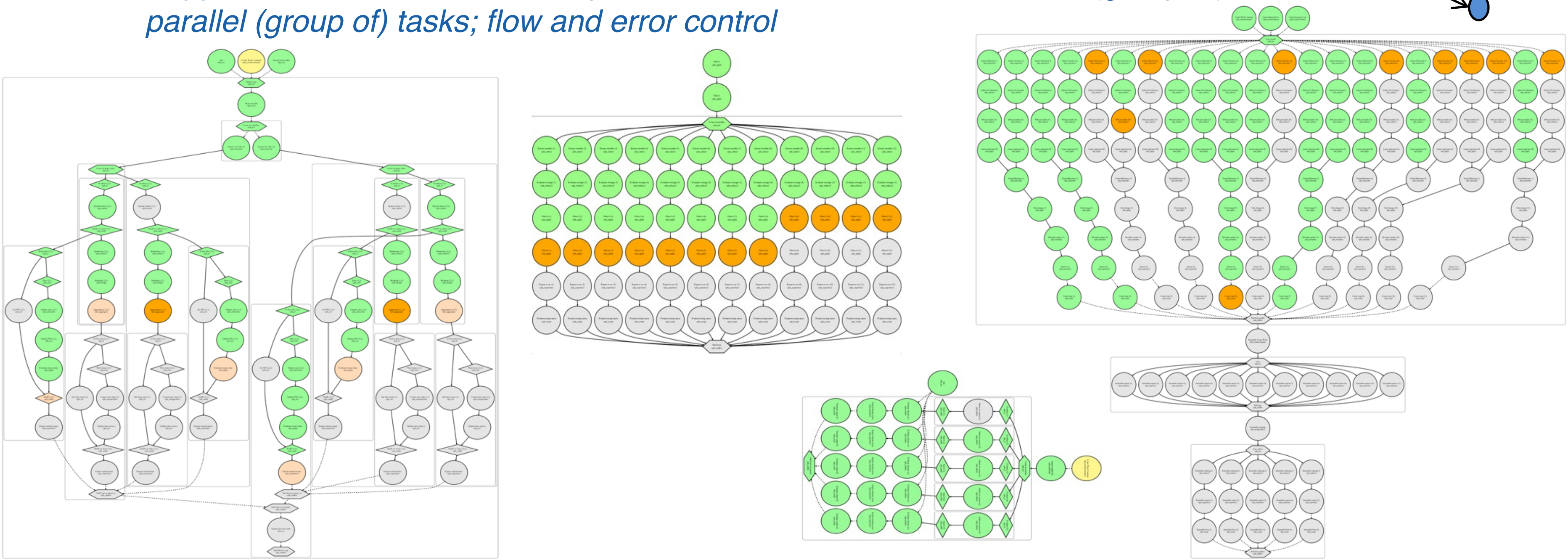
Practical PyOphidia tutorial

Analytics workflows

Ophidia supports the execution of complex workflows of operators.



- Defines a **JSON representation** for the workflow DAG specification
- Supports different constructs: *dependencies; massive tasks; iterative (group of) tasks; parallel (group of) tasks; flow and error control*



C. Palazzo, A. Mariello, S. Fiore, A. D'Anca, D. Elia, D. N. Williams, G. Aloisio, "A Workflow-Enabled Big Data Analytics Software Stack for eScience", HPCS 2015, pp. 545-552

Session outline

Introduction to Big Data, HPDA and data challenges in eScience

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Practical PyOphidia tutorial

Programmatic support for data science applications

PyOphidia is a Python module to interact with the Ophidia framework.

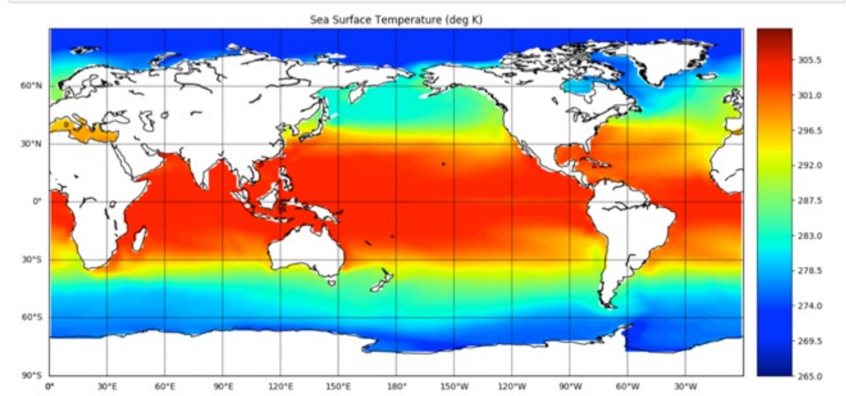
It provides a programmatic access to Ophidia features, allowing:

- *Submission of commands to the Ophidia Server and retrieval of the results*
- *Management of (remote) data objects in the form of datacubes*
- *Easy exploitation from Jupyter Notebooks and integration with other Python modules*

```
from PyOphidia import cube, client
cube.Cube.setclient(read_env=True)

mycube =
cube.Cube.importnc(src_path='/public/data/ecas_training
/file.nc', measure='tos', imp_dim='time',
import_metadata='yes', ncores=5)
mycube2 = mycube.reduce(operation='max',ncores=5)
mycube3 = mycube2.rollup(ncores=5)
data = mycube3.export_array()

mycube3.exportnc2(output_path='/home/test',
export_metadata='yes')
```



Export result to NetCDF file

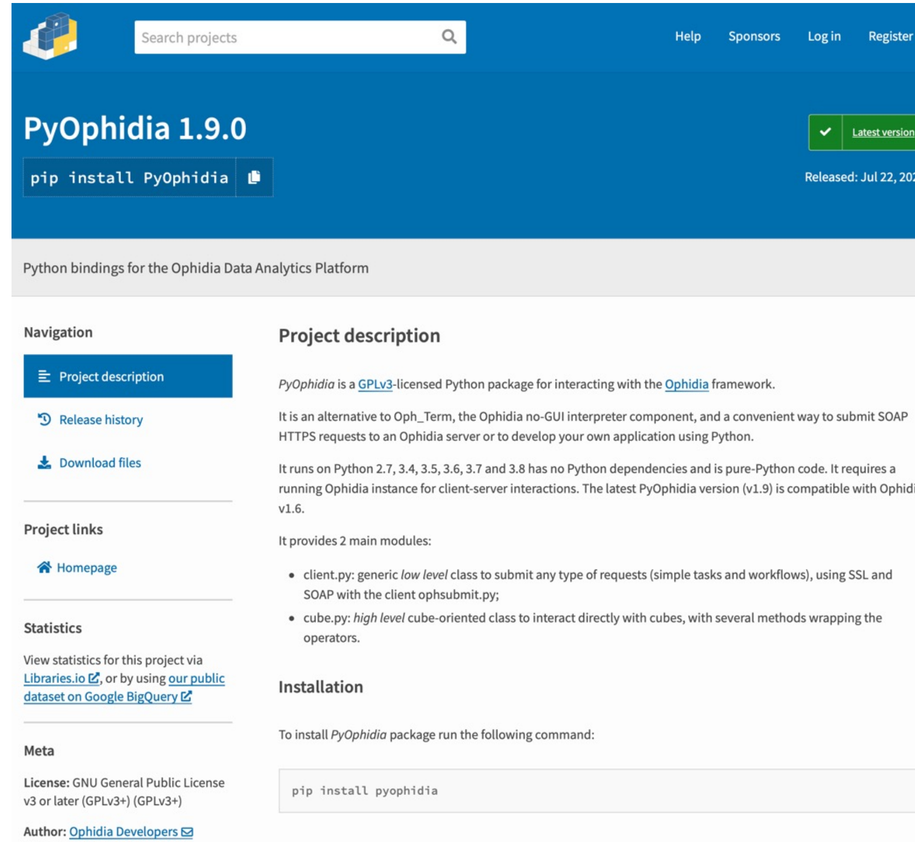
```
]: mycube3.exportnc2(output_path='/home/' + cube.Cube.client.username,export_metadata='yes')
```

The PyOphidia library

PyOphidia implements two main classes:

- ***Client class****: supports submissions of Ophidia commands and workflows, as well as sessions management from Python (like the Ophidia Terminal)*
- ***Cube class****: provides datacube type abstraction (object-oriented approach) and methods to manipulate, process and get information on cubes objects and it builds on the client class*

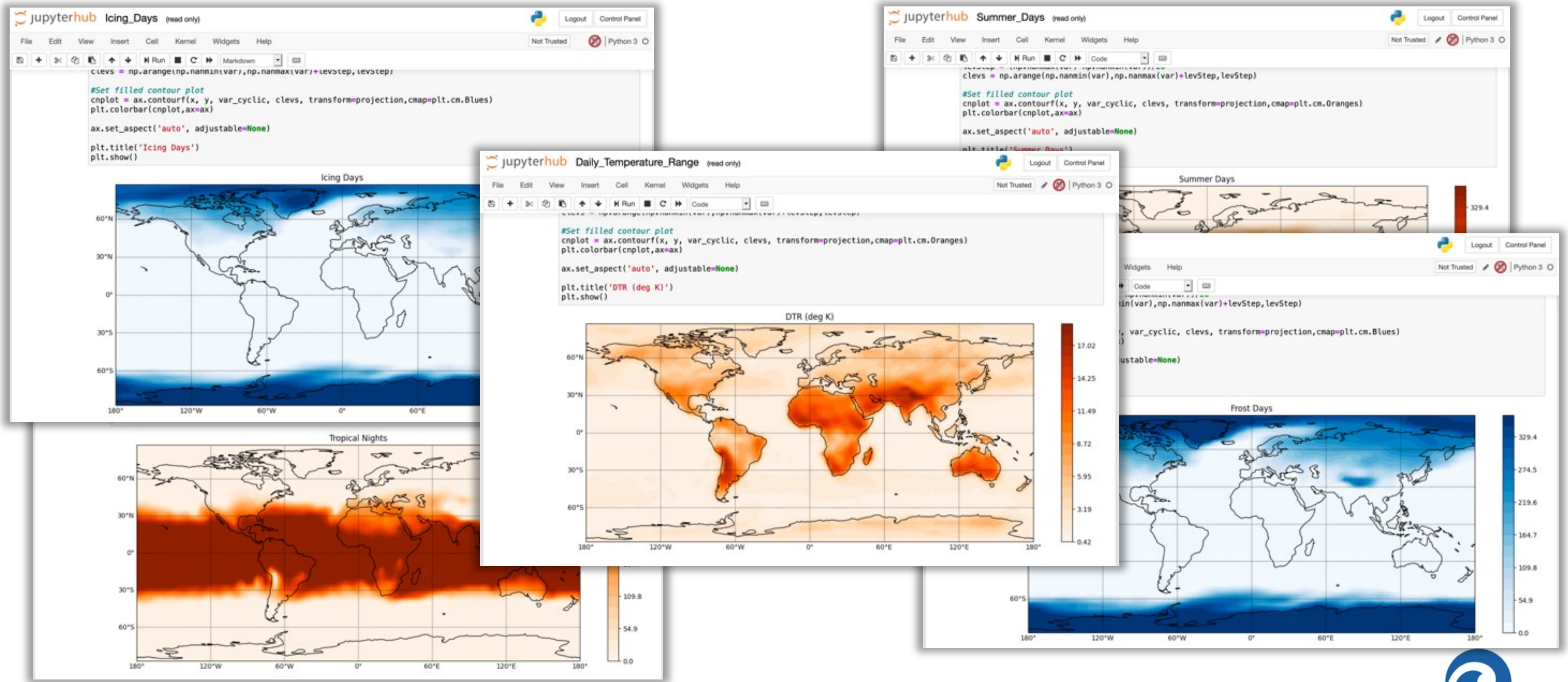
While the cube module provides a user-friendly interface, the client module allows a finer specification of the operators.



https://pypi.org/project/PyOphidia/
https://anaconda.org/conda-forge/pyophidia

Interactive climate data analytics

PyOphidia can be combined with other Python libraries (e.g., cartopy, matplotlib) and Notebooks for interactive prototyping, computation and visualization of climate indices



Python and HPC infrastructure transparency

PyOphidia class hides the HPC environment complexity

```
In [ ]: from PyOphidia import cube, client
        cube.Cube.setclient(read_env=True)

In [ ]: cube.Cube.cluster(action='deploy',host_partition='test_partition',nhost=4)

In [ ]: myCube = cube.Cube(src_path='/work/ophidia/tests/tasmax_day_CMCC-CESM_rcp85.nc',
            measure='tasmax', import_metadata='yes', imp_dim='time', description='Max Temps',
            nfrag=16, nhosts=4,
            host_partition='test2',
            ncores=2, nthreads=8
            )

In [ ]: myCube2 = maxtemp.apply(
            query="oph_predicate('oph_float','oph_int',measure,'x-298.15','>0','1','0')",
            ncores=2, nthreads=8
        )

In [ ]: myCube3 = myCube2.subset(subset_filter=1, subset_dims='time')

In [ ]: pythonData = myCube3.export_array(show_time='yes')

In [ ]: print(pythonData)

In [ ]: cube.Cube.cluster(action='undeploy',host_partition='test_partition')
```

Python and HPC infrastructure transparency

PyOphidia class hides the HPC environment complexity

In [ ]:
```
from PyOphidia import cube, client
cube.Cube.setclient(read_env=True)
```

Dynamic I/O & Analytics nodes allocation

In [ ]:
```
cube.Cube.cluster(action='deploy',host_partition='test_partition',nhost=4)
```

In [ ]:
```
myCube = cube.Cube(src_path='/work/ophidia/tests/tasmax_day_CMCC-CESM_rcp85.nc',
    measure='tasmax', import_metadata='yes', imp_dim='time', description='Max Temps',
    nfrag=16, nhosts=4,
    host_partition='test2',
    ncores=2, nthreads=8
    )
```

Data partitioning and distribution

Framework operator parallelism

In [ ]:
```
myCube2 = maxtemp.apply(
    query="oph_predicate('oph_float','oph_int',measure,'x-298.15','>0','1','0')",
    ncores=2, nthreads=8
)
```

In [ ]:
```
myCube3 = myCube2.subset(subset_filter=1, subset_dims='time
```

Ophidia-notebook data translation and transfer

In [ ]:
```
pythonData = myCube3.export_array(show_time='yes')
```

In [ ]:
```
print(pythonData)
```

In [ ]:
```
cube.Cube.cluster(action='undeploy',host_partition='test_partition')
```

I/O & Analytics nodes undeployment

What have we learned so far?

Joining HPC and data analytics is an enabling factor for scientific applications

Several challenges for climate (scientific) data management and analytics should be addressed: novel and efficient software solution are required

Overview of the Ophidia HPDA framework main aspects and how it addresses data analytics challenges for scientific analysis

- *Datacube abstraction for multi-dimensional scientific (climate) data*
- *Scalable architecture, data distribution, parallel operators*

PyOphidia Python module provides a high-level interface for parallel data management and analysis abstracting from the infrastructure complexity

Next: practical tutorial with PyOphidia

Environment setup

Requirements: *Docker, git CLI* and a *web browser*

For the tutorial we are using the *Ophidia all-in-one training container* from DockerHub*:*

```
docker pull ophidiabigdata/ophidia-training:latest
```

Further information at: [*https://hub.docker.com/r/ophidiabigdata/ophidia-training*](https://hub.docker.com/r/ophidiabigdata/ophidia-training)

Retrieve the tutorial/demo material from *GitHub:*

```
git clone https://github.com/ESiWACE/hpda-vis-training.git
```

Download the data required for the training:

```
cd hpda-vis-training/SummerSchool2021/HPDA_Ophidia
./get_data.sh
```

You should now see two CMIP5 NetCDF files under the git repository folder.

Start the environment

From the same folder start the container, binding the tutorial material repo path ($PWD):

```
docker run --rm -it -v $PWD:/home/ophidia/notebooks
ophidiabigdata/ophidia-training:latest
```

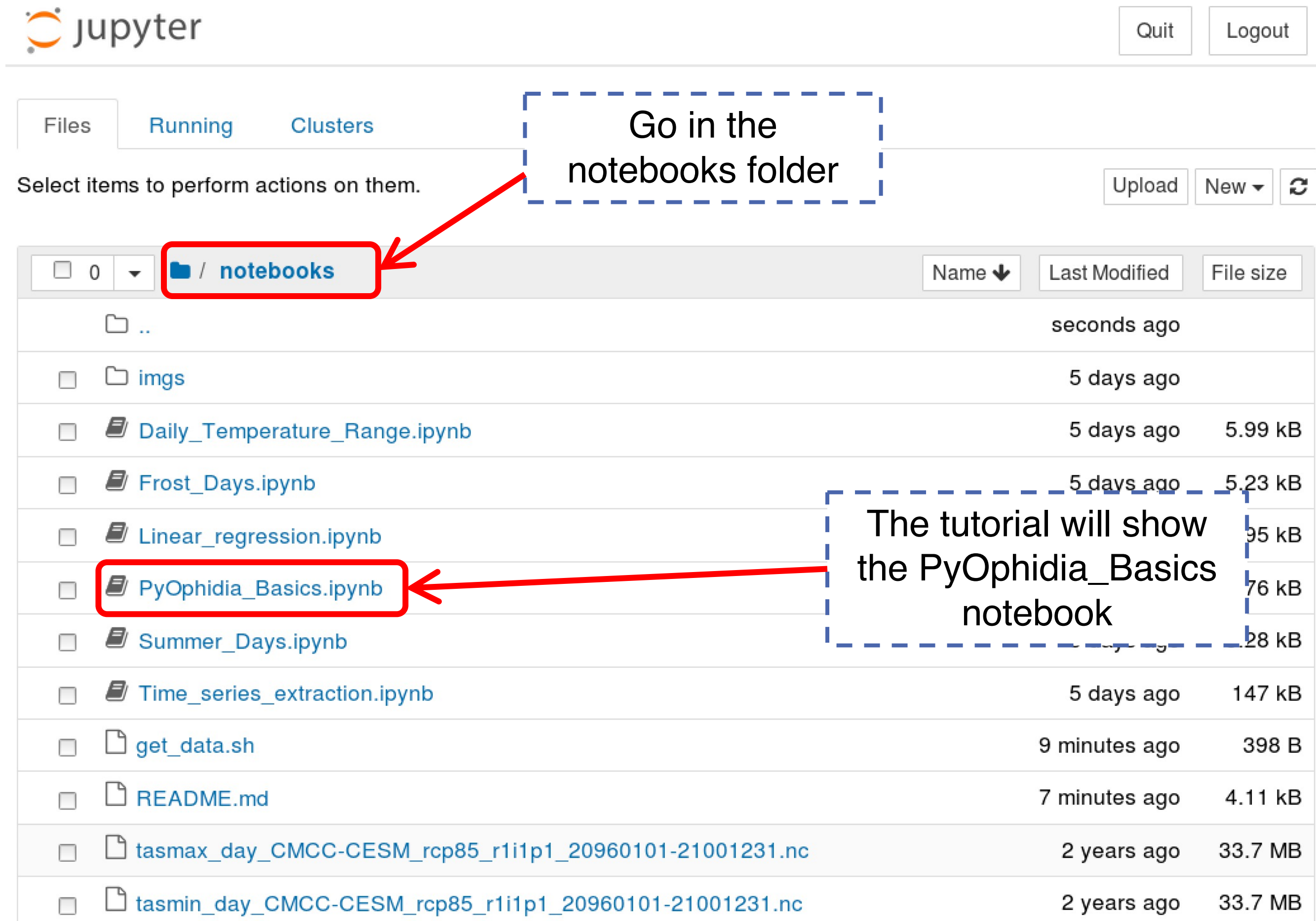
This container includes the full Ophidia software stack, a Jupyter Notebook server and a set of scientific Python modules.

If started correctly you should get something like the following messages in the terminal:

```
[I 20:43:36.116 NotebookApp] Writing notebook server cookie secret to
/usr/local/ophidia/.local/share/jupyter/runtime/notebook_cookie_secret
[I 20:43:36.539 NotebookApp] Serving notebooks from local directory: /home/ophidia
[I 20:43:36.539 NotebookApp] Jupyter Notebook 6.4.0 is running at:
[I 20:43:36.540 NotebookApp] http://172.17.0.2:8888/
[I 20:43:36.540 NotebookApp] Use Control-C to stop this server and shut down all kernels
(twice to skip confirmation).
```

Now copy the URL showed by the message (e.g., http://172.17.0.2:8888/) in your browser to open the Jupyter Notebook UI and type '*ophidia*' as password.

Run the tutorial notebooks



References and further readings

- *D. A. Reed and J. Dongarra. (2015). Exascale computing and big data. Commun. ACM 58, 7 (July 2015), 56–68.*
- *Asch, M., et al. (2018). Big data and extreme-scale computing: Pathways to convergence-toward a shaping strategy for a future software and data ecosystem for scientific inquiry. Int. J. High Perform. Comput. Appl., 32(4), 435-479.*
- *S. Fiore, et al. (2013). Ophidia: Toward Big Data Analytics for eScience. ICCS 2013, volume 18 of Procedia Computer Science, pp. 2376-2385.*
- *S. Fiore, et al. (2014). "Ophidia: A Full Software Stack for Scientific Data Analytics", proc. of the 2014 Int. Conference on High Performance Computing & Simulation (HPCS 2014), pp. 343-350.*
- *S. Fiore, D. Elia, C. Palazzo, F. Antonio, A. D'Anca, I. Foster and G. Aloisio (2019), "Towards High Performance Data Analytics for Climate Change", ISC High Performance 2019. Lecture Notes in Computer Science, vol. 11887, pp. 240-257.*
- *D. Elia, S. Fiore and G. Aloisio, "Towards HPC and Big Data Analytics Convergence: Design and Experimental Evaluation of a HPDA Framework for eScience at Scale," in IEEE Access, vol. 9, pp. 73307-73326, 2021*
- *D. Elia, et al. (2016). "An in-memory based framework for scientific data analytics". In Proc. of the ACM Int. Conference on Computing Frontiers (CF '16), pp. 424-429.*
- *C. Palazzo, et al. (2015), "A Workflow-Enabled Big Data Analytics Software Stack for eScience", HPCS 2015, pp. 545-552*
- *A. D'Anca, et al. (2017), "On the Use of In-memory Analytics Workflows to Compute eScience Indicators from Large Climate Datasets," 2017 17th IEEE/ACM Int. Symposium on Cluster, Cloud and Grid Computing (CCGRID), pp. 1035-1043.*
- *S. Fiore, et al. (2016). "Distributed and cloud-based multi-model analytics experiments on large volumes of climate change data in the earth system grid federation eco-system". In Big Data (Big Data), 2016 IEEE Int. Conference on. IEEE. pp. 2911-2918.*

Questions?

ESiWACE2 *has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823988*

Ophidia website: [*http://ophidia.cmcc.it*](http://ophidia.cmcc.it)

Contact: *donatello.elia [at] cmcc.it*

ophidia-info [at] cmcc.it

Interested in learning more?

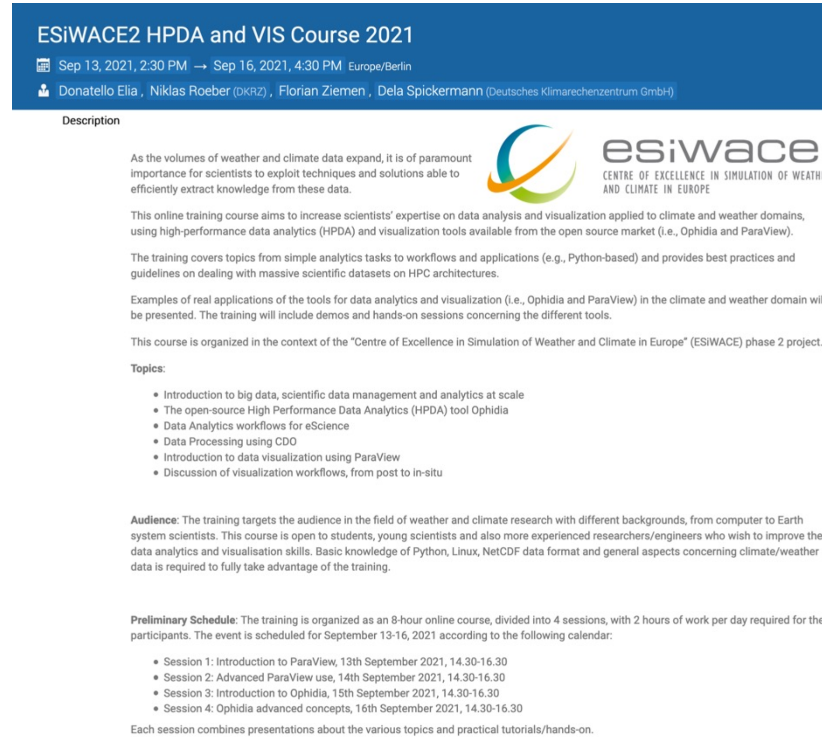
ESiWACE2 online training course on High-Performance Data Analytics (HPDA) and Visualisation

The course will consist of four 2-hour online sessions from the ***13th to the 16th of September 2021 (2:30pm - 4:30pm CEST)****.*

It provides insights into data analysis and visualization applied to climate and weather domains, using HPDA and visualization tools available from the open source market. Examples of real applications of these tools (i.e., Ophidia and ParaView) in the climate and weather domain will be given.

To attend the course, register ***not later than the 8th of September*** *at: https://indico.dkrz.de/e/esiwace-hpda-vis-2021*

Additional information about the training is available at: https://www.esiwace.eu/events/hpda-vis-training-2021



ESiWACE2 HPDA and VIS Course 2021

Sep 13, 2021, 2:30 PM → Sep 16, 2021, 4:30 PM Europe/Berlin

Donatello Elia , Niklas Roeber (DKRZ) , Florian Ziemen , Dela Spickermann (Deutsches Klimarechenzentrum GmbH)

Description

As the volumes of weather and climate data expand, it is of paramount importance for scientists to exploit techniques and solutions able to efficiently extract knowledge from these data.

This online training course aims to increase scientists' expertise on data analysis and visualization applied to climate and weather domains, using high-performance data analytics (HPDA) and visualization tools available from the open source market (i.e., Ophidia and ParaView).

The training covers topics from simple analytics tasks to workflows and applications (e.g., Python-based) and provides best practices and guidelines on dealing with massive scientific datasets on HPC architectures.

Examples of real applications of the tools for data analytics and visualization (i.e., Ophidia and ParaView) in the climate and weather domain will be presented. The training will include demos and hands-on sessions concerning the different tools.

This course is organized in the context of the "Centre of Excellence in Simulation of Weather and Climate in Europe" (ESiWACE) phase 2 project.

Topics:

- Introduction to big data, scientific data management and analytics at scale
- The open-source High Performance Data Analytics (HPDA) tool Ophidia
- Data Analytics workflows for eScience
- Data Processing using CDO
- Introduction to data visualization using ParaView
- Discussion of visualization workflows, from post to in-situ

Audience: The training targets the audience in the field of weather and climate research with different backgrounds, from computer to Earth system scientists. This course is open to students, young scientists and also more experienced researchers/engineers who wish to improve their data analytics and visualisation skills. Basic knowledge of Python, Linux, NetCDF data format and general aspects concerning climate/weather data is required to fully take advantage of the training.

Preliminary Schedule: The training is organized as an 8-hour online course, divided into 4 sessions, with 2 hours of work per day required for the participants. The event is scheduled for September 13-16, 2021 according to the following calendar:

- Session 1: Introduction to ParaView, 13th September 2021, 14.30-16.30
- Session 2: Advanced ParaView use, 14th September 2021, 14.30-16.30
- Session 3: Introduction to Ophidia, 15th September 2021, 14.30-16.30
- Session 4: Ophidia advanced concepts, 16th September 2021, 14.30-16.30

Each session combines presentations about the various topics and practical tutorials/hands-on.