

Introduction to HPDA and Ophidia

Donatello Elia, Fabrizio Antonio, Alessandro D'Anca

Fondazione Centro Euro-Mediterraneo sui Cambiamenti Climatici (CMCC), Lecce, Italy



Ophidia

ENCCS/CMCC workshop:
*Training on HPDA for climate data with the
Ophidia framework*

11 November 2021

Agenda of the training

10:00-10:10 Welcome

10:10-10:40 Introduction to HPDA and Ophidia

10:40-11:15 Tutorial about PyOphidia basic usage

11:15-11:20 Short break

11:20-12:00 Hands-on on interactive analysis with PyOphidia

12:00 -13:00 Lunch break

13:00-13:40 Data analytics workflows with Ophidia

13:40-14:15 Tutorial about workflow building in Ophidia

14:15-14:20 Short break

14:20-15:00 Hands-on on data analytics workflows



Session outline

Introduction to HPDA and data challenges in eScience

Overview of the Ophidia HPDA framework

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

Ophidia Python bindings: PyOphidia

DEMO: Tutorial about PyOphidia usage

HANDS-ON: Data analytics examples with PyOphidia

Disclaimer: this material reflects only the authors' view, and the EU-Commission is not responsible for any use that may be made of the information it contains.



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 parallelise 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*



Session outline

Introduction to HPDA and data challenges in eScience

Overview of the Ophidia HPDA framework

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

Ophidia Python bindings: PyOphidia

DEMO: Tutorial about PyOphidia usage

HANDS-ON: Data analytics examples with PyOphidia



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

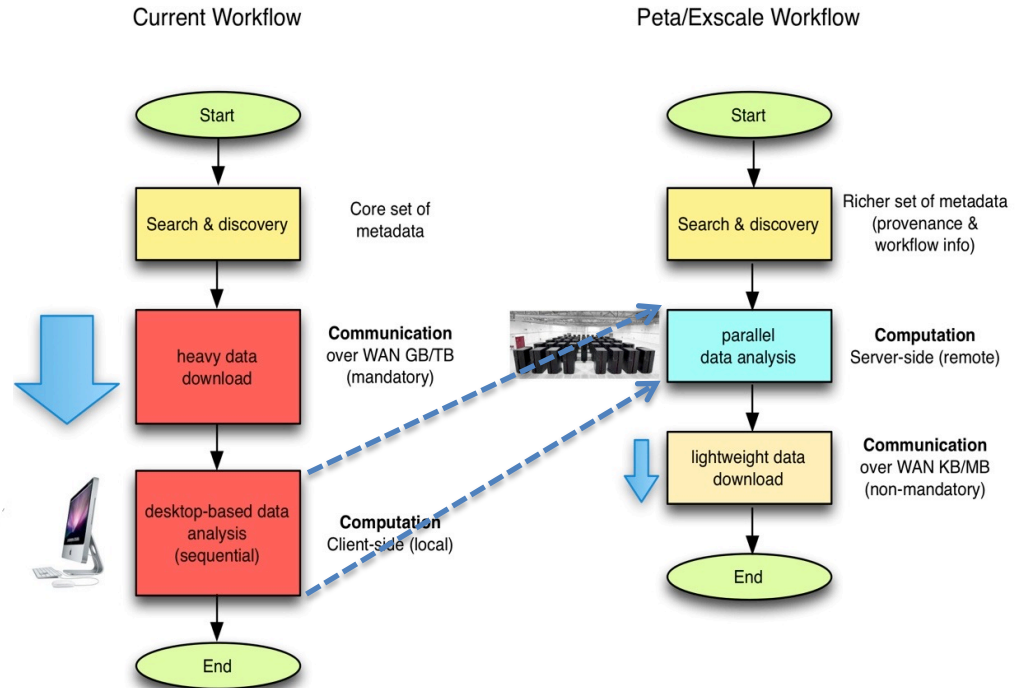
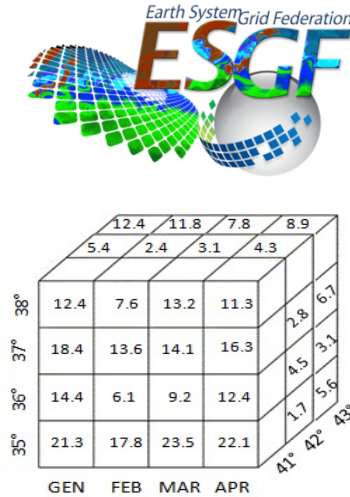
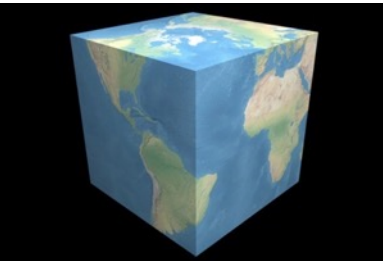
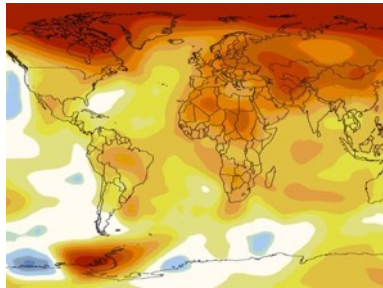


S. Fiore, D. Elia, C. Palazzo, F. Antonio, A. D'Anca, I. Foster, G. Aloisio, "Towards High Performance Data Analytics for Climate Change", ISC High Performance 2019, LNCS Springer, 2019



A paradigm shift

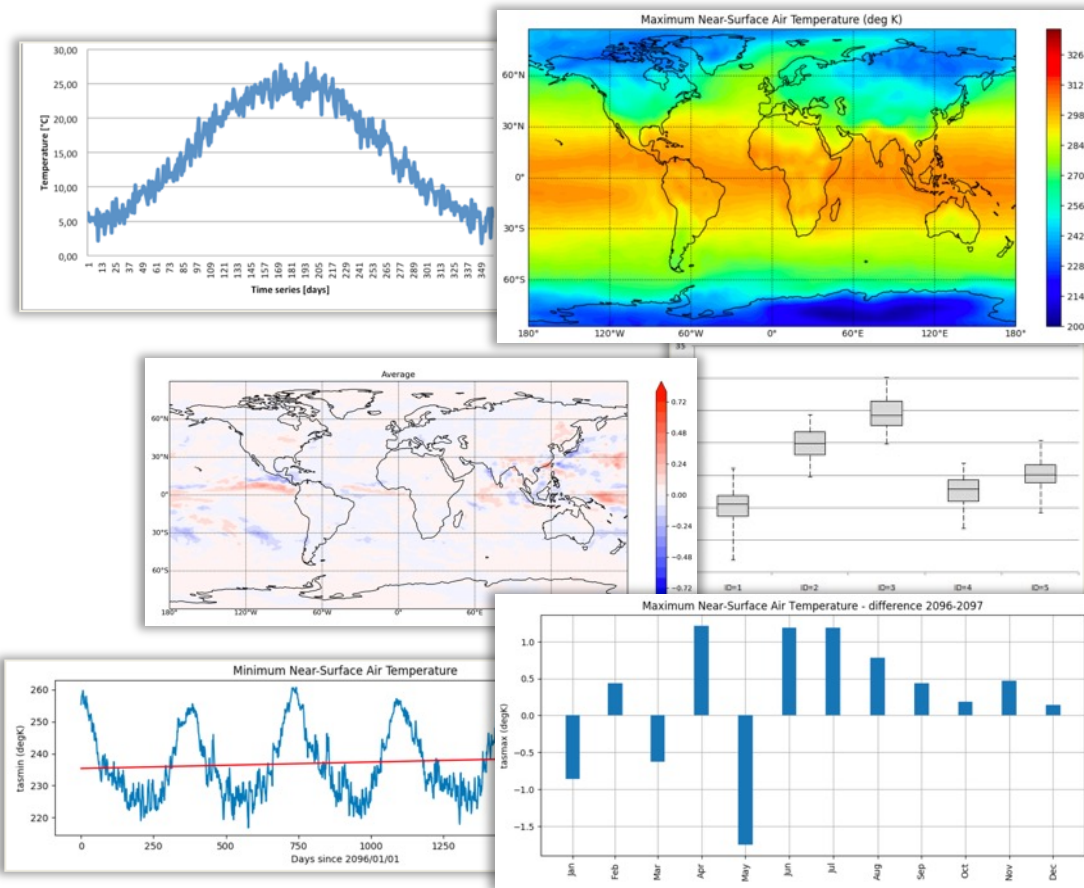
Volume, variety, velocity are key challenges for big data in general and for climate sciences in particular. Client-side, sequential and disk-based workflows are three limiting factors for the current scientific data analysis tools.



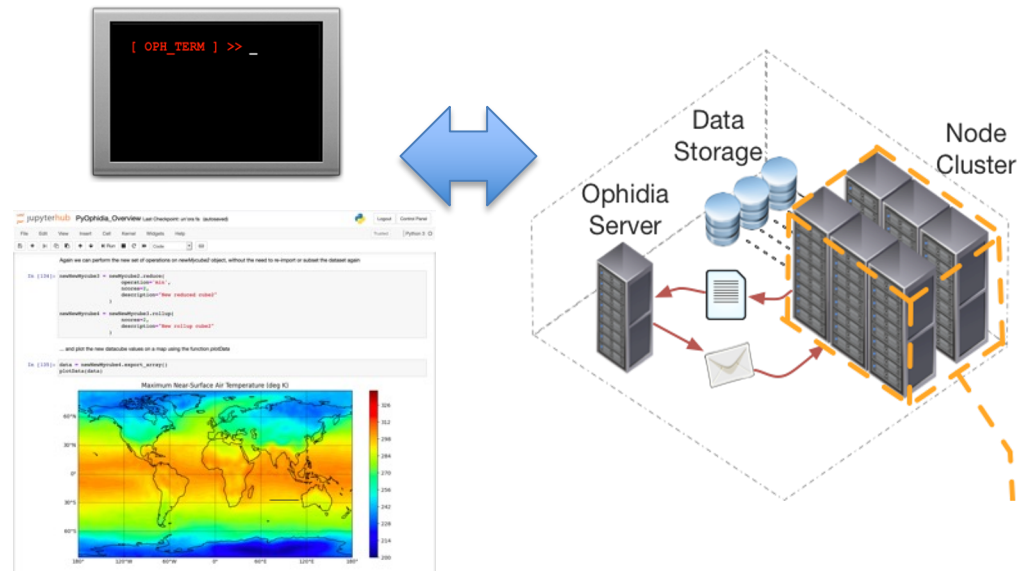
Data analytics requirements and use cases

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

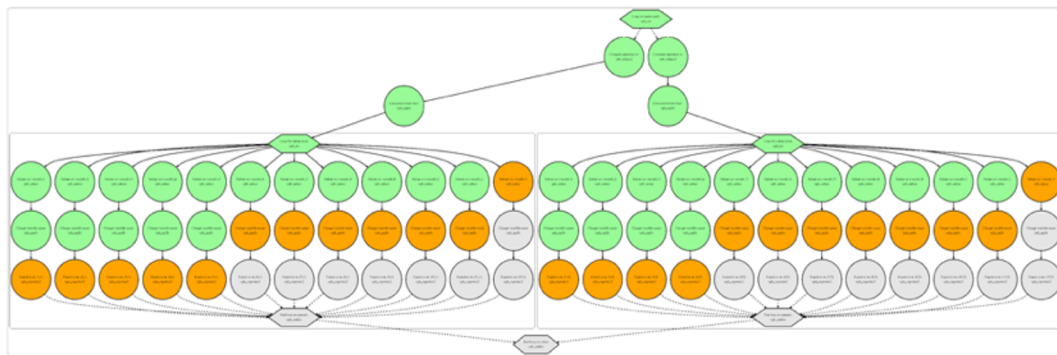


Oph_Term: a terminal-like commands interpreter serving as a client for the Ophidia framework

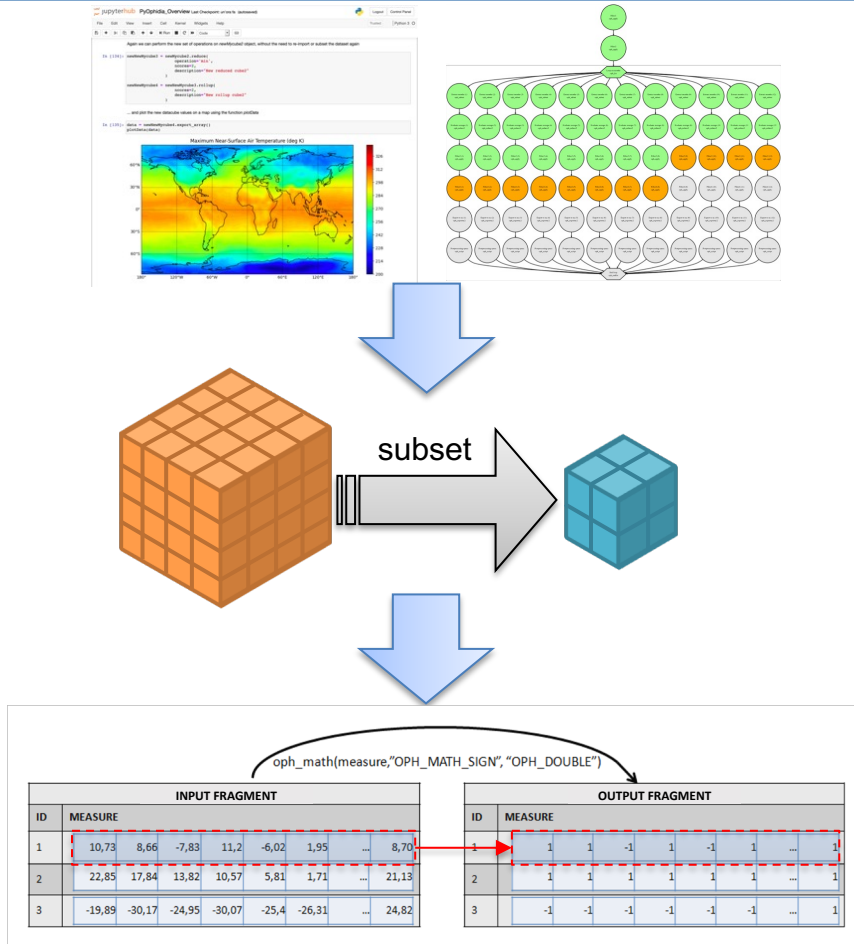
PyOphidia: a Python interface for datacube management & analytics with Ophidia

Multiple execution modes:

- *Interactive analysis (e.g. notebooks)*
- *Python applications*
- *Workflows of operators*
- *Async/sync execution*



Granularity of operations in Ophidia



Workflows/applications: combine multiple Ophidia Operators to compute from complex experiments (e.g., multi-model analysis) to simple indicators (e.g., Summer Days)

Ophidia Operators: datacube-level operations on multi-dimensional data. Both data and metadata. Some examples: subsetting, aggregation, comparison

Ophidia Primitives: low-level functions applied on the single binary arrays of the datacube fragments. Some examples: time series analysis, array transformations



Some international projects exploiting Ophidia



esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER
AND CLIMATE IN EUROPE



eFlows4HPC

is-enes
INFRASTRUCTURE FOR THE EUROPEAN NETWORK
FOR EARTH SYSTEM MODELLING



EOSC-hub



EU Brazil Cloud Connect
EU Brazil Cloud Computing for Science



EUROPE - BRAZIL
COLLABORATION OF BIG DATA
SCIENTIFIC RESEARCH THROUGH
CLOUD-CENTRIC APPLICATIONS



Climate Information Portal



INDIGO - DataCloud



Session outline

Introduction to HPDA and data challenges in eScience

Overview of the Ophidia HPDA framework

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

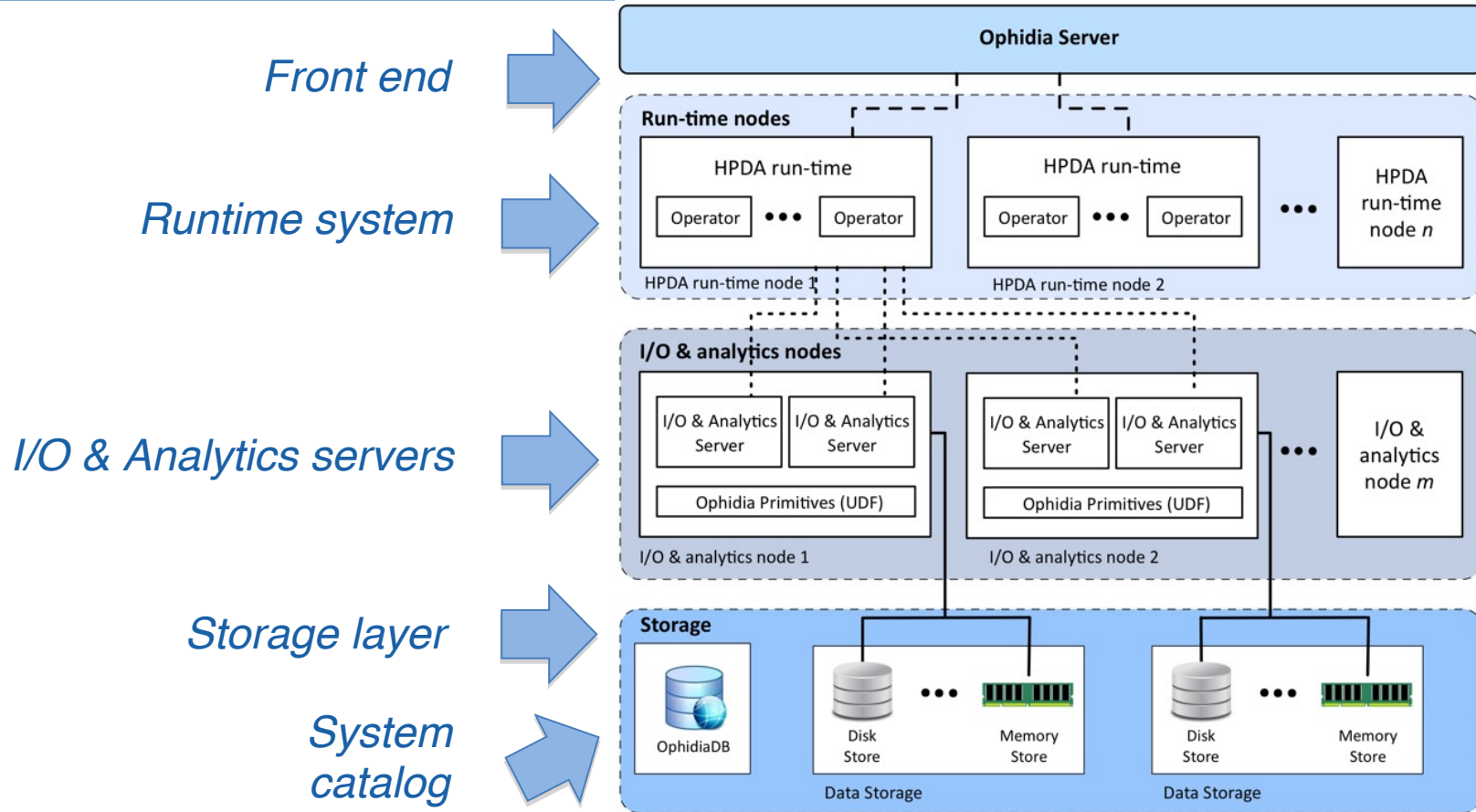
Ophidia Python bindings: PyOphidia

DEMO: Tutorial about PyOphidia usage

HANDS-ON: Data analytics examples with PyOphidia



Ophidia architecture: overview



Ophidia architecture: storage layer & model

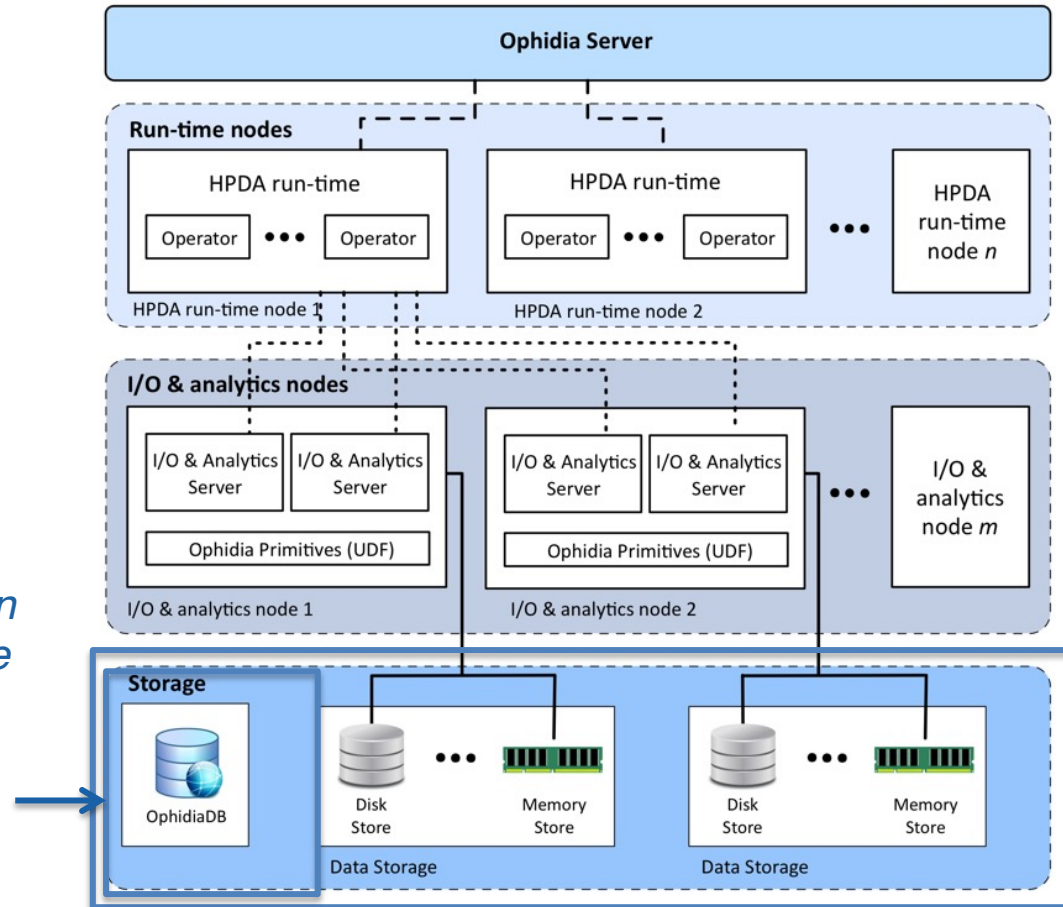
Distributed hardware resources to manage storage

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

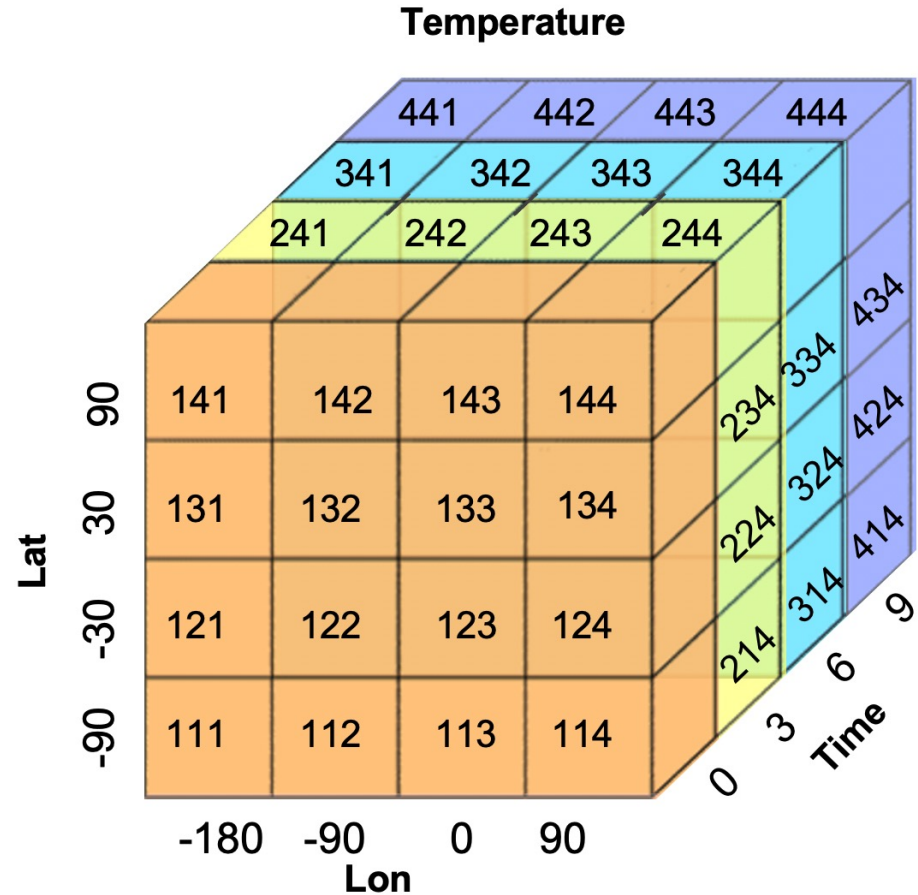
Data partitioned in a hierarchical fashion over the storage according to the storage model & partitioning schema

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



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

```
oph_importnc  
src_path=test.nc;measure=Temperature;  
imp_dim=time;ncores=2;nfrags=2;
```

lat	lon	Temperature			
		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

NetCDF



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:
explicit dimensions

```
oph_importnc  
src_path=test.nc;measure=Temperature;  
imp_dim=time;ncores=2;nfrags=2;
```

lat	lon	Temperature			
		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

NetCDF

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,  
      ...  
}
```

Mapped to a single
unique key

```
oph_importnc  
src_path=test.nc;measure=Temperature;  
imp_dim=time;ncores=2;nfrags=2;
```

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

NetCDF

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

```
oph_importnc  
src_path=test.nc;measure=Temperature;  
imp_dim=time;ncores=2;nfrags=2;
```

		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

Data reorganised
based on implicit and
explicit dimensions

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

Table horizontally
partitioned in multiple
fragments

```
oph_importnc  
src_path=test.nc;measure=Temperature;  
imp_dim=time;ncores=2;nfrags=2;
```

lat	lon	Temperature			
		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

lat	lon	Temperature			
		time[0]	time[1]	time[2]	time[3]
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

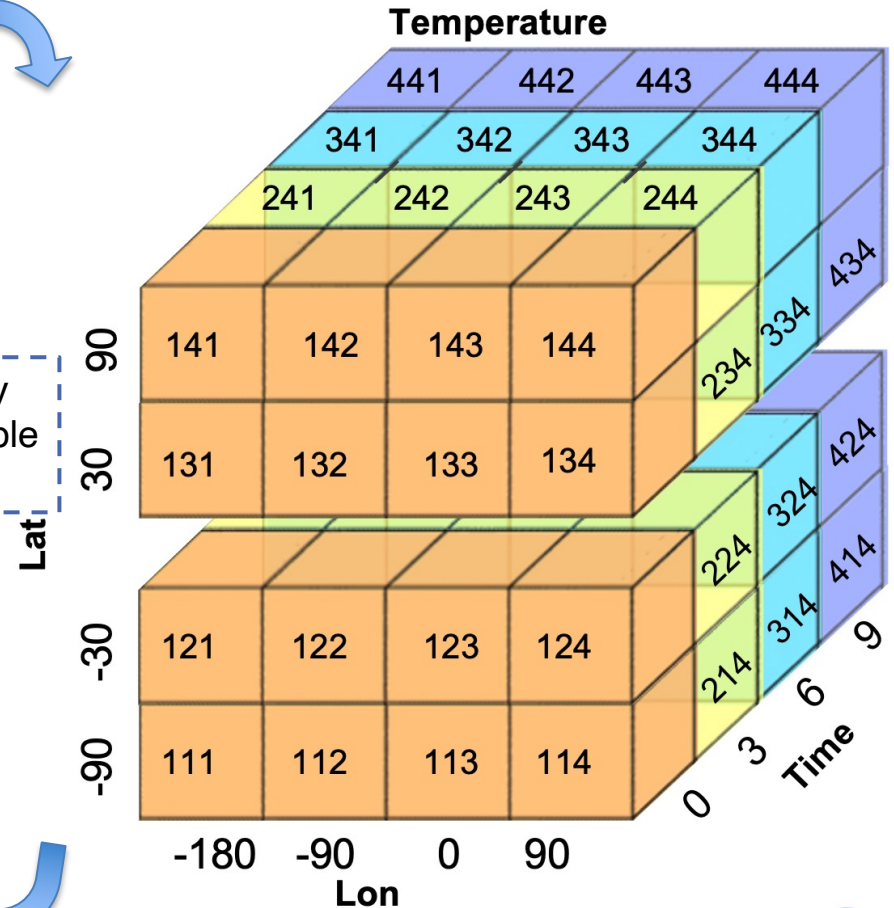
Ophidia



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,  
      ...  
}
```

Table horizontally
partitioned in multiple
fragments



NetCDF

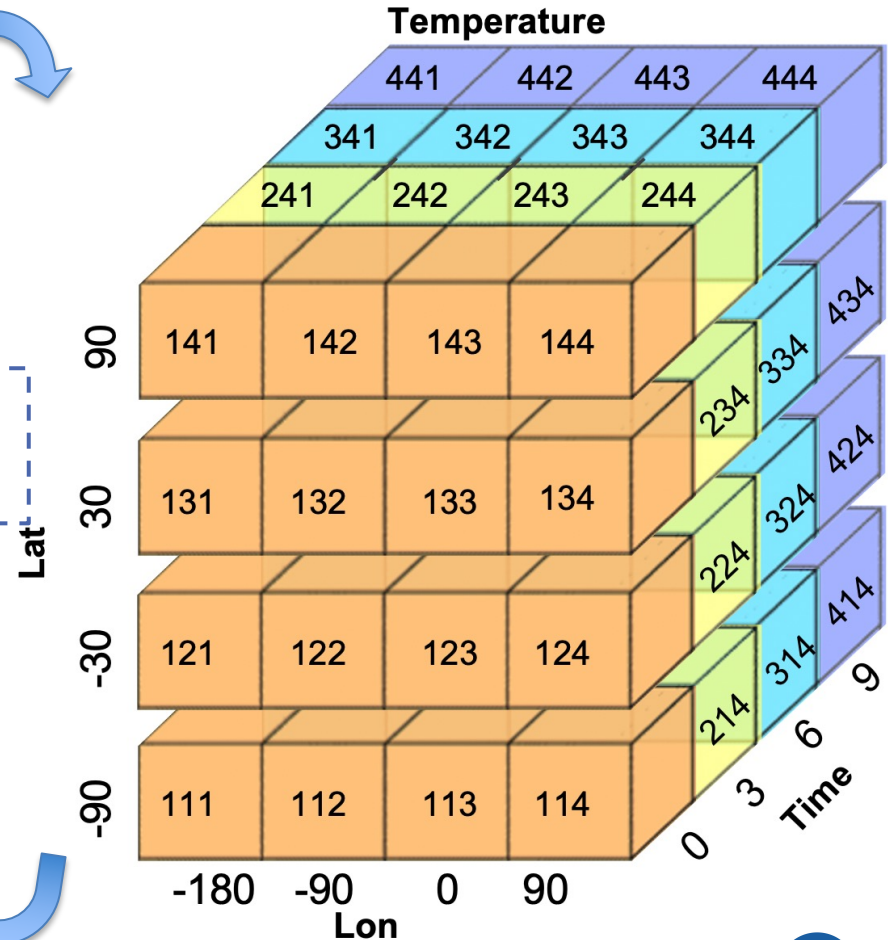


From NetCDF to Ophidia

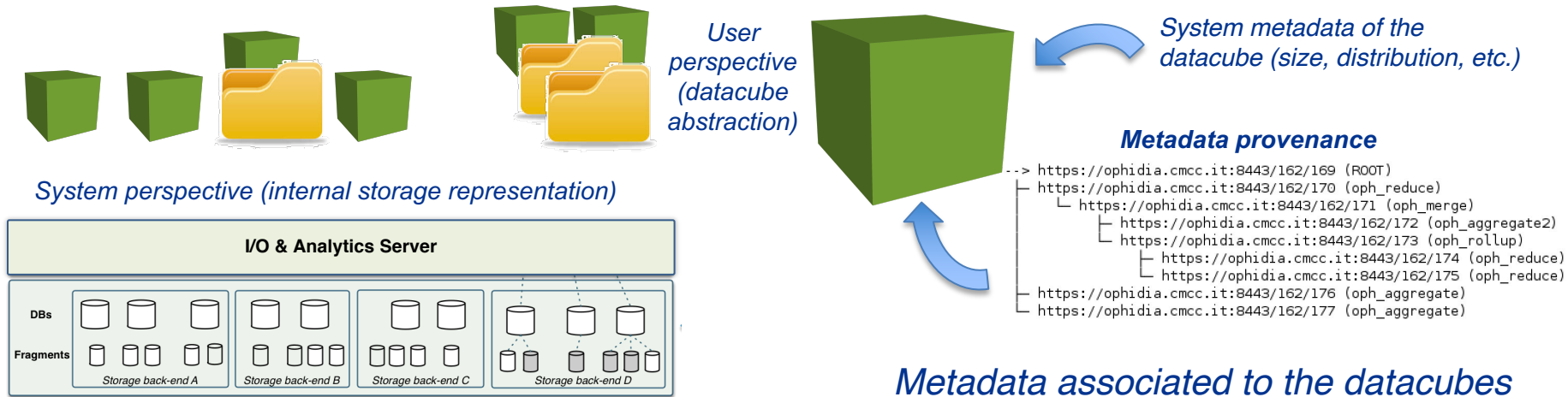
```
netcdf test {  
  dimensions:  
    lat = 4 ;  
    lon = 4 ;  
    time = UNLIMITED // (4 currently) ;  
  variables:  
    double lon(lon) ;  
    double lat(lat) ;  
    double time(time) ;  
    float Temperature(time, lat, lon) ;  
  data:  
    lon = -180, -90, 0, 90 ;  
    lat = -90, -30, 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,  
      ...  
}
```

Fragmentation can
be increased for
parallel analysis

NetCDF



Data abstraction: cube space perspective



Metadata associated to the datacubes

CMD	BEHAVIOUR
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

Searching results				
Id	Variable	Key	Type	Value
736 930 68	tas	standard_name	text	air_temperature
736 930 69	tas	long_name	text	Air Temperature
736 930 70	tas	comment	text	This is sampled synoptically.
736 930 71	tas	units	text	K
736 930 72	tas	original_name	text	temp2



Ophidia architecture: I/O & Analytics layer

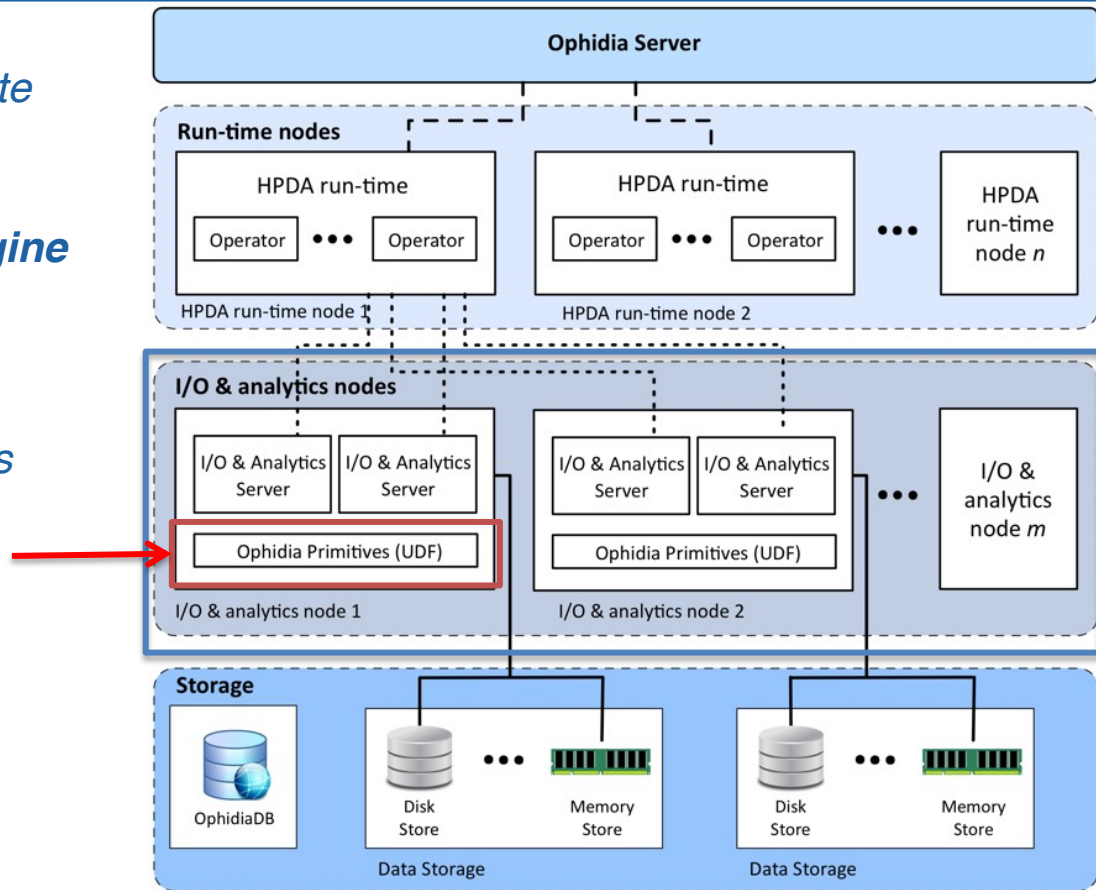
*Multiple **I/O & analytics nodes** execute one or more servers*

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

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

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

Servers can transparently interface to different storage back-ends



Ophidia array-based primitives

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

- data summarisation, 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'))
```



Array-based primitives: nesting support

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

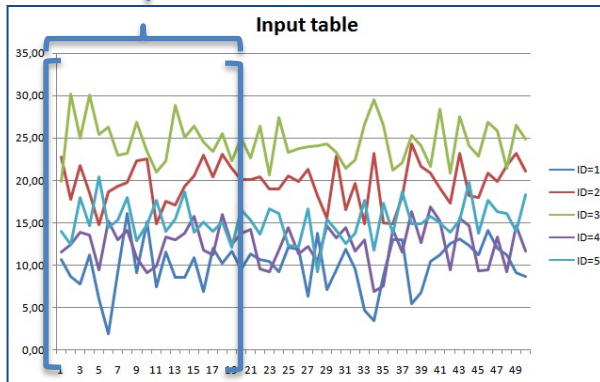
Single chunk or fragment (input)

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

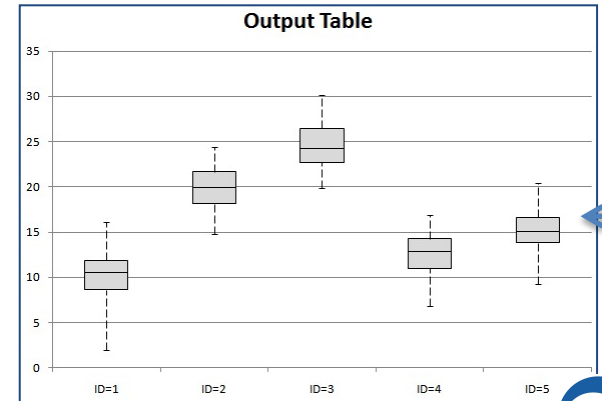
Single chunk or fragment (output)

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

subarray(measure, 1,18)



Scientific representation



Ophidia architecture: HPDA runtime layer

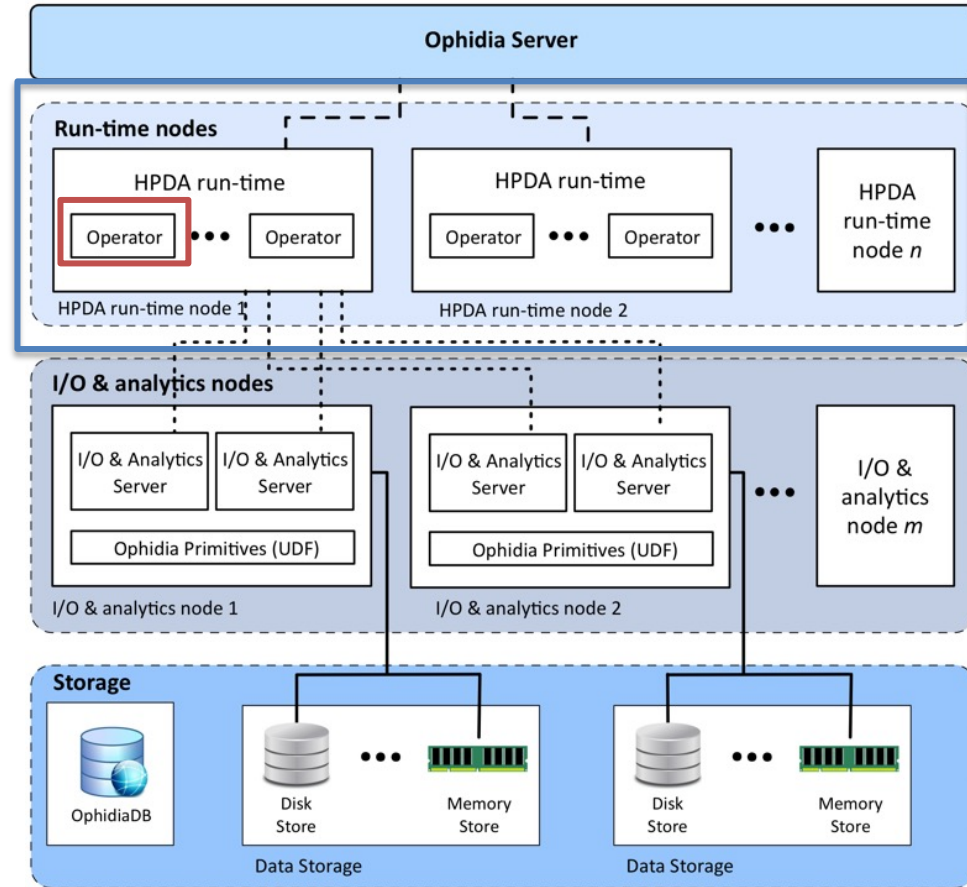
The Ophidia HPDA runtime system can be executed with **multiple processes/threads** and **distributed over multiple nodes**

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**



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_MERGE_CUBES
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



“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;sessionid=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
```

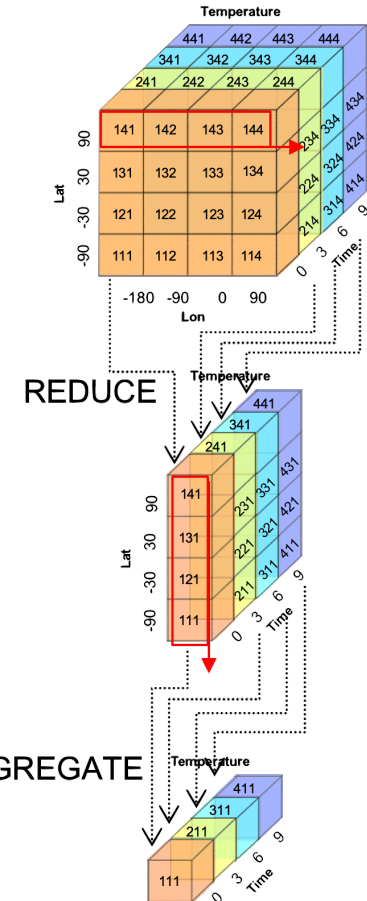
```
[12..3289] >> oph_aggregate operation=avg;ncores=2;nthreads=2;  
[Request]:  
operator=oph_aggregate;operation=avg;ncores=2;nthreads=2;sessionid=http://127.0.0.1/ophidia/sessions/127028404128222463341617004437753289/experiment;exec_mode=sync;cube=http://127.0.0.1/ophidia/418/12722;cwd=/;cdd=/;host_partition=auto;
```

```
[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

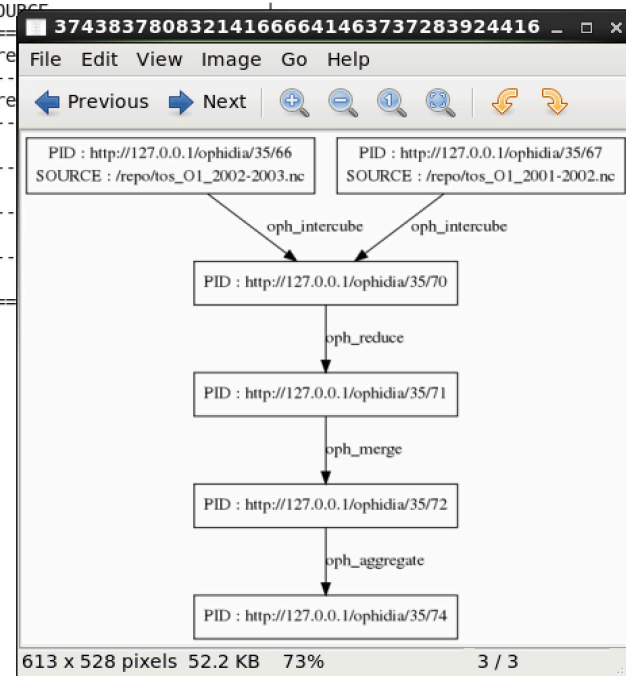
Directed Graph DOT string :

```

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_01_2002-2003.nc\n"]
    5         [label="PID : http://127.0.0.1/ophidia/35/67\nSOURCE : /repo/tos_01_2001-2002.nc\n"]

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

```



613 x 528 pixels 52.2 KB 73%

3 / 3

Ophidia architecture: front-end layer

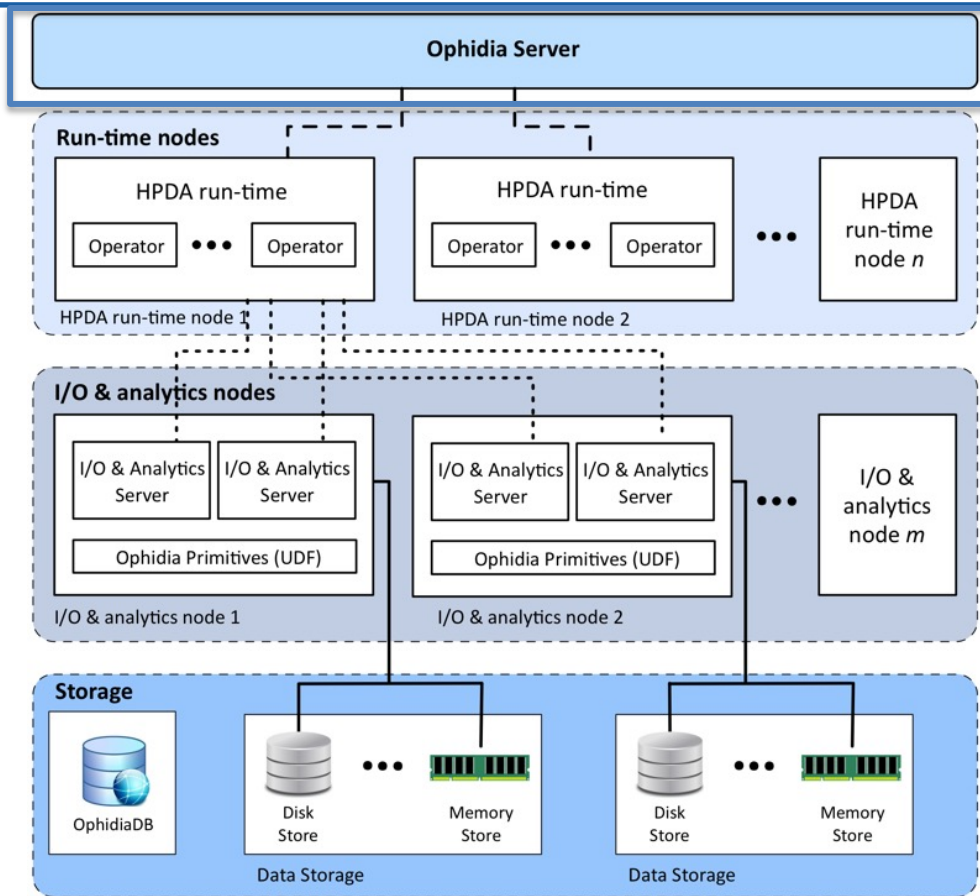
The **Ophidia Server** is the **multi-interface** server front-end

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



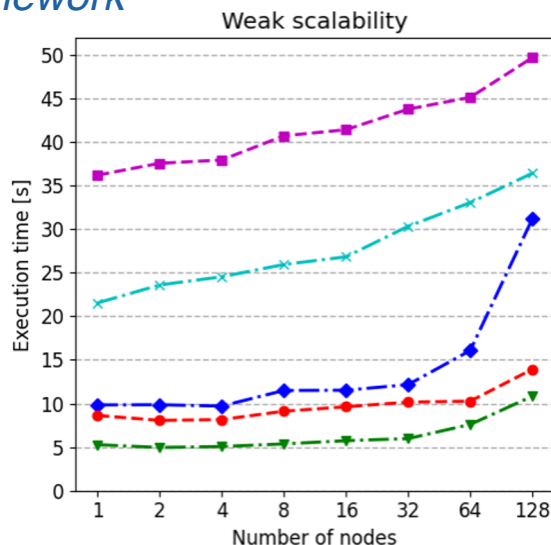
Ophidia HPDA framework benchmark

Goal: benchmarking, tuning and optimisation over a large-scale HPC machine of the Ophidia HPDA framework

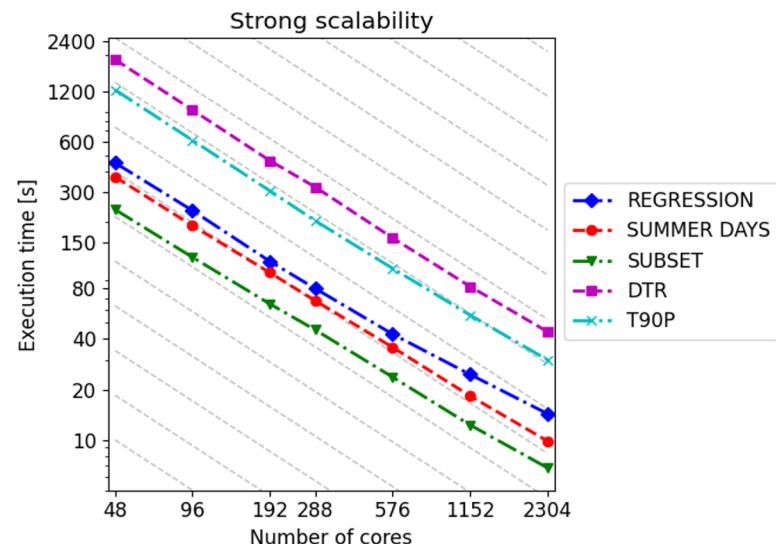


Evaluate the scalability of Ophidia analytics kernels on a few thousands of cores:

- various **strong** and **weak** scalability tests run
- **good scalability** in most the cases until **3k cores**



Data size per node: 67GiB



Data size fixed: 3.2TiB

We acknowledge PRACE for awarding access to MareNostrum 4 at Barcelona Supercomputing Center (BSC), Spain and the support provided by BSC (PRACE resources for CoE, in the context of ESiWACE).



Session outline

Introduction to HPDA and data challenges in eScience

Overview of the Ophidia HPDA framework

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

Ophidia Python bindings: PyOphidia

DEMO: Tutorial about PyOphidia usage

HANDS-ON: Data analytics examples with PyOphidia



Programmatic support for data science applications

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

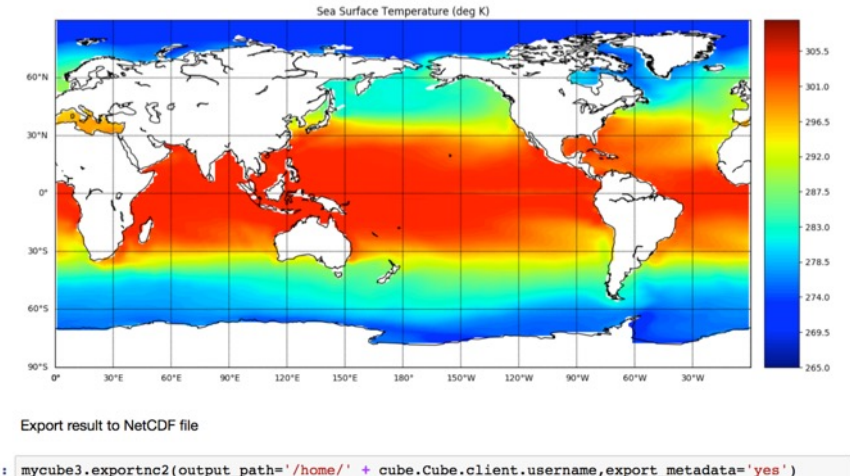
It provides a programmatic access to Ophidia features, allowing:

- *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)

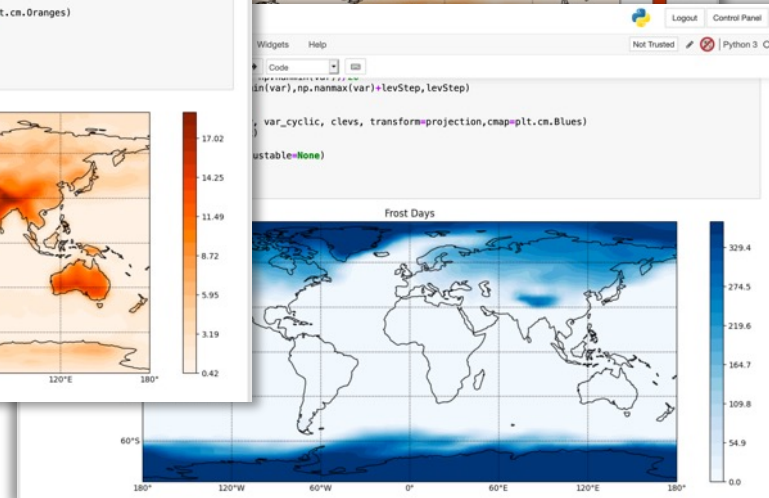
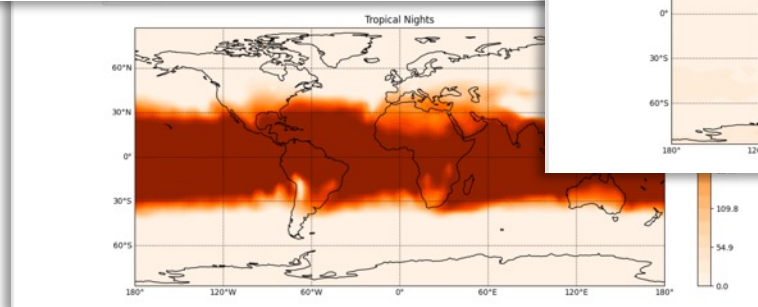
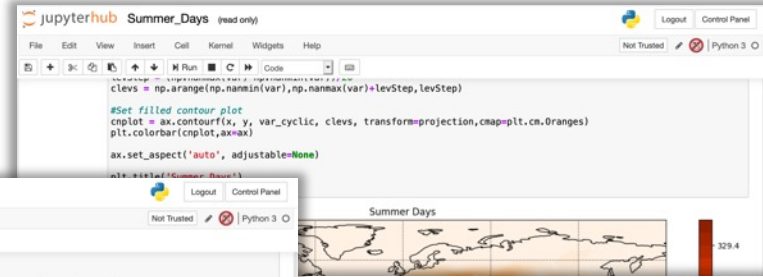
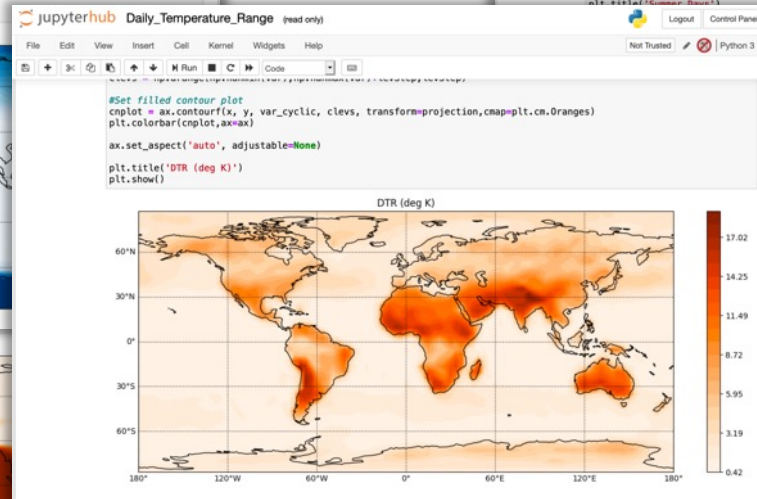
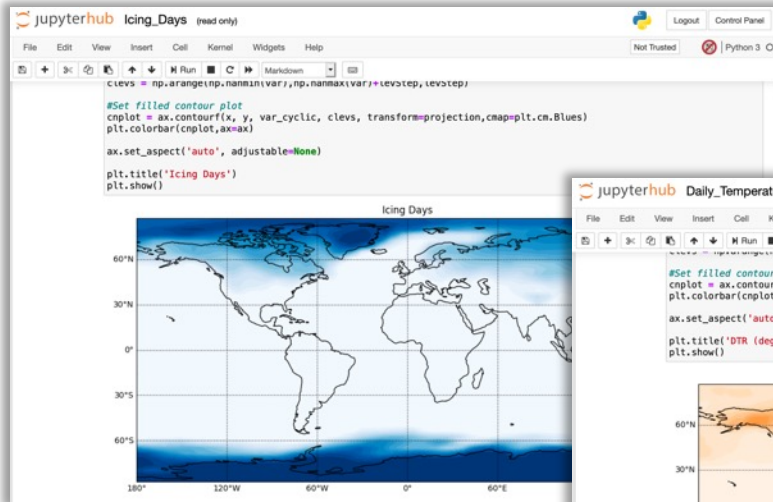
mycube =
cube.Cube.importnc(src_path='/public/data/ecas_training
/file.nc', measure='tos', imp_dim='time',
import_metadata='yes', ncores=5)
mycube2 = mycube.reduce(operation='max', ncores=5)
mycube3 = mycube2.rollup(ncores=5)
data = mycube3.export_array()

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



Interactive climate data analytics

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



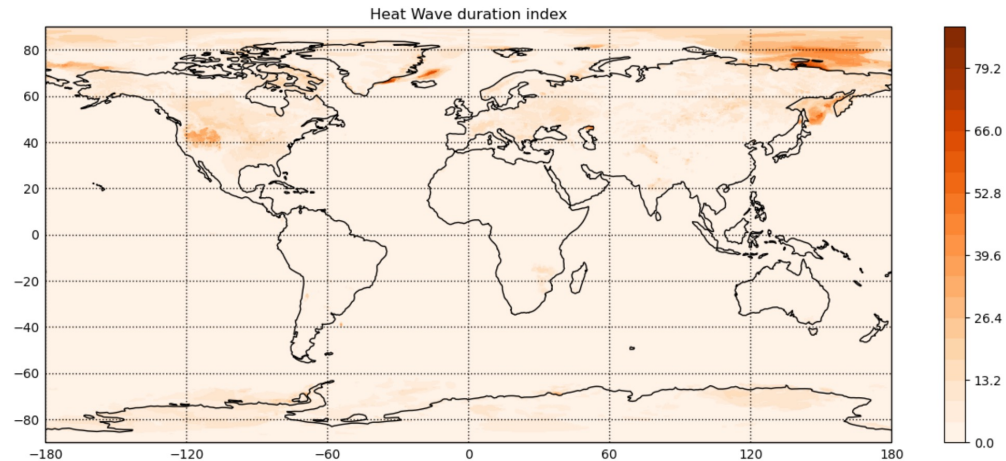
Ophidia in eFlows4HPC project

eFlows4HPC – Enabling dynamic and Intelligent workflows in the future EuroHPC ecosystem

Create a workflow software stack and an additional set of services to enable the integration of HPC simulations and modelling with big data analytics and machine learning in scientific and industrial applications

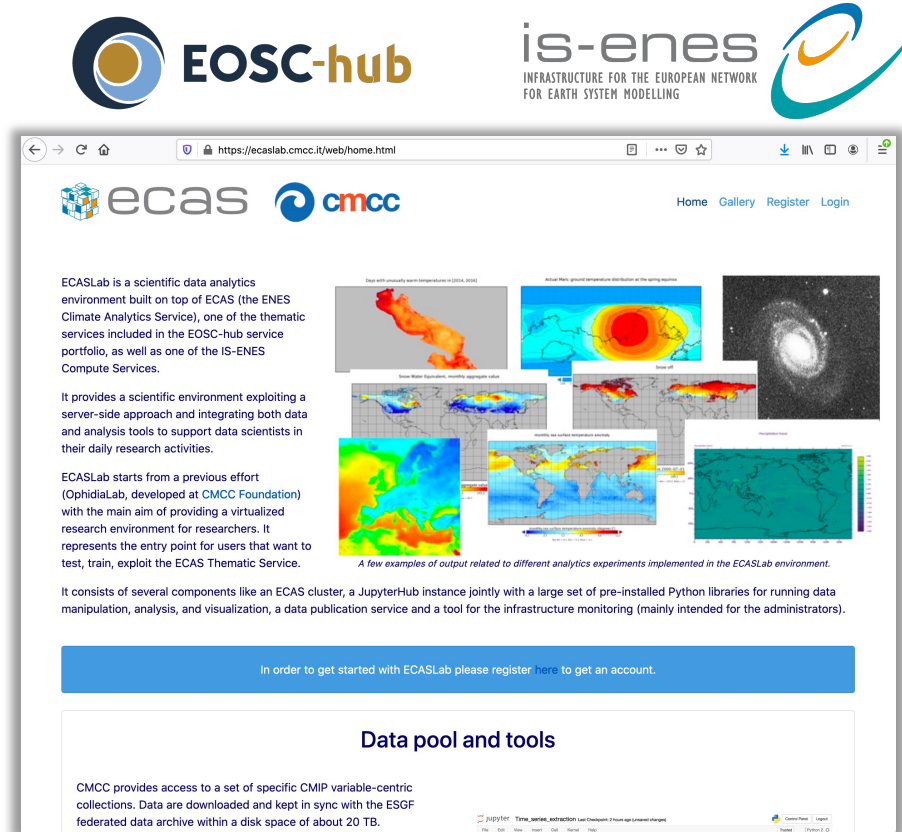
Ophidia is one of the software components of the eFlows4HPC stack:

- It is being used in the Earth System Model workflow through the PyOphidia module:
 - Pre-processing of large volumes of climate data
 - Development of extreme climate indices: HWDI, HWFI, etc.



ENES Climate Analytics Service (ECAS)

- *ECAS was developed as one of the EOSC-Hub Thematic Services and represents one of IS-ENES3 compute services*
- ECAS builds on top of the *Ophidia HPDA framework*, integrated with components from INDIGO-DataCloud, EUDAT and EGI
- Integrates computing resources with datasets and data analytics tools
- It provides a user-friendly environment based on Jupyter Notebooks, well-known Python modules and a ready-to-use Ophidia instance



ECAS @ CMCC <https://ecaslab.cmcc.it>



What have we learned so far?

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

Challenges for efficient 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: Demo and hands-on with PyOphidia



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



Acknowledgements

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



eFlows4HPC this project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway



IS-ENES3 has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 824084



Thank you!

Questions?

More about Ophidia?

Ophidia website: <http://ophidia.cmcc.it>

GitHub repo: <https://github.com/OphidiaBigData>

Contact: *ophidia-info [at] cmcc.it*

Twitter channel: <https://twitter.com/OphidiaBigData>

