ESiWACE2 HPDA & Vis Training 2021

High-Perfomance Data Analytics in eScience with the Ophidia framework

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Session 3 15 September 2021



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: Introduction to PyOphidia

HANDS-ON: Data analytics examples with PyOphidia

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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

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High Performance Data Analytics for eScience

- o Computational science modeling and data analytics are both crucial in scientific research
 - o 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 (<u>http://ophidia.cmcc.it</u>) 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





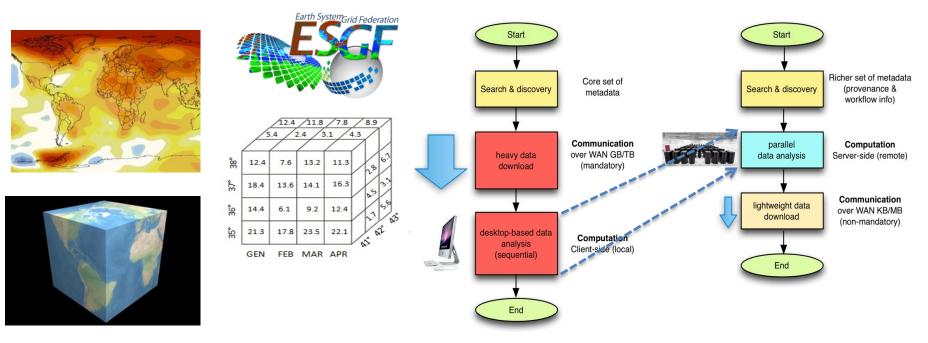
S. Fiore, D. Elia, C. Palazzo, F. Antonio, A. D'Anca, I. Foster, G. Aloisio, "Towards High Performance Data Analytics for Climate Change", ISC High Performance 2019, LNCS Springer, 2019



6

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.



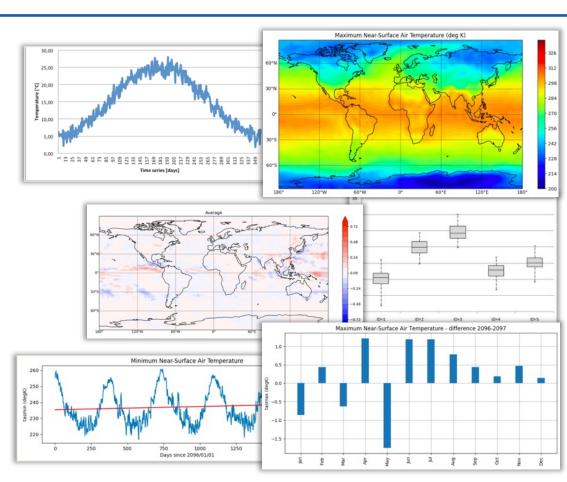
S. Fiore, A. D'Anca, C. Palazzo, I. Foster, D. N. Williams, G. Aloisio, "Ophidia: toward bigdata analytics for eScience", ICCS2013 Conference, Procedia Elsevier, 2013



Data analytics requirements and use cases

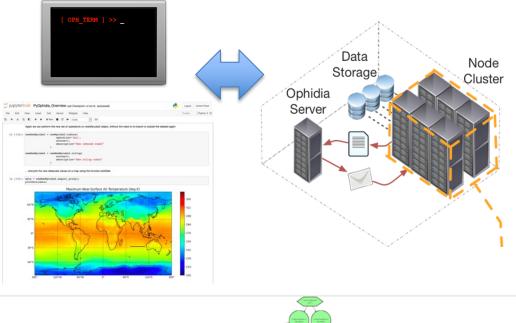
Requirements and needs focus on:

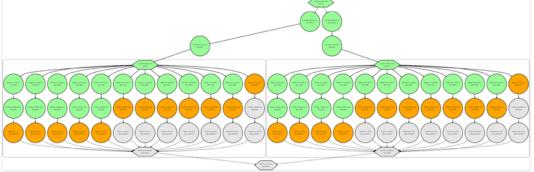
- > Time series analysis
- Data subsetting
- > Model intercomparison
- Multi-model means
- > Massive data reduction
- Data transformation
- Parameter sweep experiments
- > Maps generation
- Ensemble analysis
- Data analytics workflow support





Server-side paradigm and execution modes





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

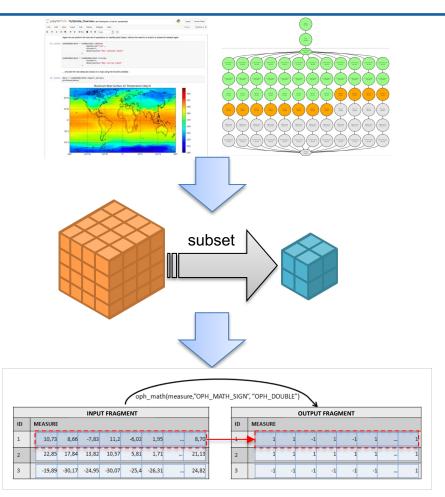
PyOphidia: a Python interface for datacube management & analytics with Ophidia

Multiple execution modes:

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



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 metadate. 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



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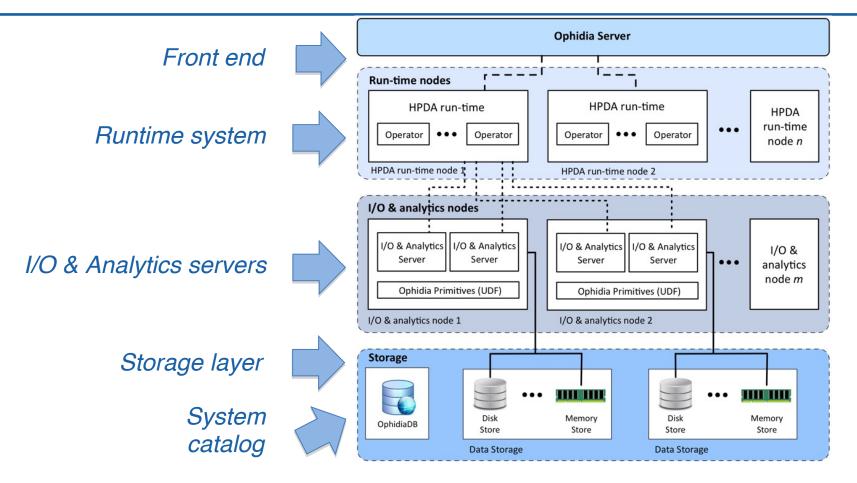
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Ophidia architecture: overview



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Ophidia architecture: storage layer & model

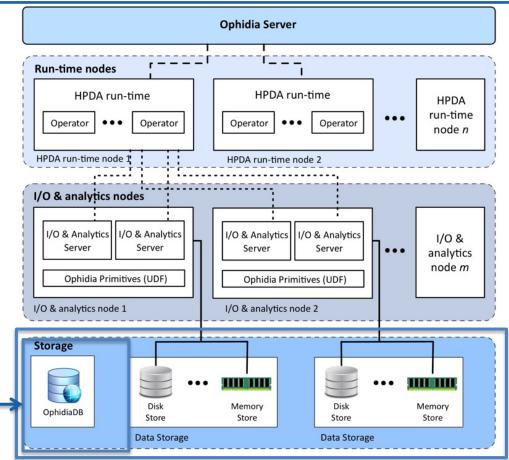
Distributed hardware resources to manage storage

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

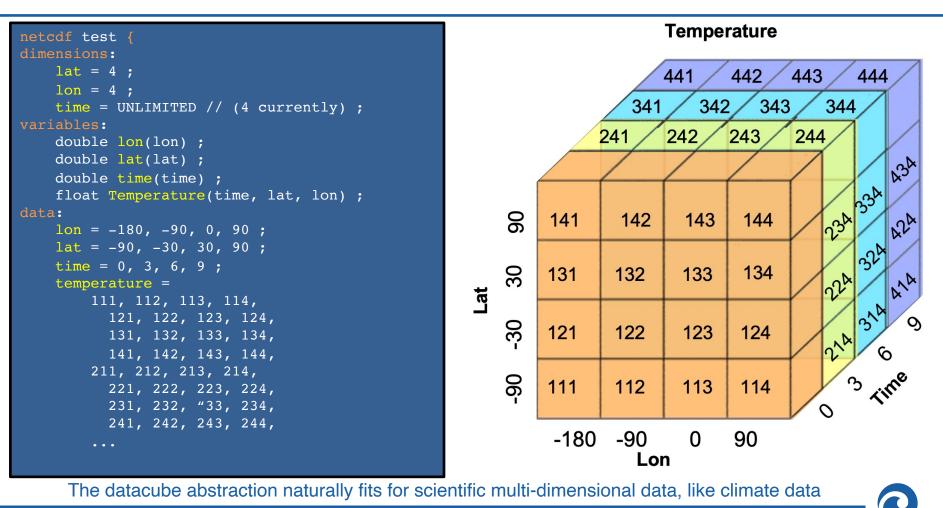
OphidiaDB is the system catalog: maps data fragmentation and tracks metadata



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



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<pre>netcdf test { dimensions: late = 4 + i </pre>	5						
lat = 4;					Tempe	rature	
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<pre>time = UNLIMITED // (4 currently) ; variables:</pre>		-90	-180	111	211	311	411
double lon(lon) ;		-90	-90	112	212	312	412
double lat(lat);		-90	0	113	213	313	413
double time(time);		-90	90	113		313	414
float Temperature(time, lat, lon);					214		
data:		-30	-180	121	221	321	421
lon = -180, -90, 0, 90;		-30	-90	122	222	322	422
lat = -90, -30, 30, 90;		-30	0	123	223	323	423
time = 0, 3, 6, 9; Defined as:		-30	90	124	224	324	424
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131, 132, 133, 134,		30	90	134	234	334	434
141, 142, 143, 144,		90	-180	141	241	341	441
211, 212, 213, 214,		90	-90	142	242	342	442
221, 222, 223, 224,		90	0	143	243	343	443
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241, 242, 243, 244,		90	90	144	244	344	444
311, 312, 313, 314,					Ophidia		
NetCDF	\sim						



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CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

<pre>netcdf test {</pre>								
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variables:				-180		211		411
<pre>double lon(lon) ;</pre>			-90	-90	112	212	312	412
<pre>double lat(lat) ;</pre>			-90	0	113	213	313	413
<pre>double time(time) ;</pre>			-90	90	114	214	314	414
float Temperature(time, lat	t, lon) ;		-30	-180	121	221	321	421
data: lon = $-180, -90, 0, 90;$			-30	-90	122	222	322	422
	Defined as:		-30	0	123	223	323	423
lat = -90, -30, 30, 90;			-30	90	124	224	324	424
<pre>time = 0, 3, 6, 9 ; temperature =</pre>	explicit dimension		30	-180	131	231	331	431
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141, 142, 143, 144,			90	-180	141	241	341	441
211, 212, 213, 214,			90	-90	142	242	342	442
221, 222, 223, 224,			90	0	143	243	343	443
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311, 312, 313, 314,						Ophidia		
						opinaia		
NetCDF		\sim						



<pre>netcdf test { dimensions: lat = 4 ; lon = 4 ;</pre>					
<pre>time = UNLIMITED // (4 currently) ;</pre>	ID		Ar	ray	
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<pre>double lat(lat) ;</pre>	3	113	213	313	413
<pre>double time(time) ;</pre>	4	114	214	314	414
<pre>float Temperature(time, lat, lon) ;</pre>	5	121	221	321	421
data:	6	122	222	322	422
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NetCDF					

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<pre>time = UNLIMITED // (4 currently)</pre>	;						
variables:		-90	-180	111	211	311	411
<pre>double lon(lon) ;</pre>		-90	-90	112	212	312	412
<pre>double lat(lat) ;</pre>		-90	0	113	213	313	413
<pre>double time(time) ;</pre>		-90	90	114	214	314	414
<pre>float Temperature(time, lat, lon)</pre>	;	-30	-180	121	221	321	421
data:			-90	122	222	322	422
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$141. 142, 143, 144, \\ 211. 212, 213, 214$		90	-180	141	241	341	441
211, 212, 213, 214, 221, 222, 223, 224,		90	-90	142	242	342	442
221, 222, 223, 224, 231, 232, 233, 234,		90	0	143	243	343	443
$231, 232, 233, 234, \\ 241, 242, 243, 244, $		90	90	144	244	344	444
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NetCDF	\sim						
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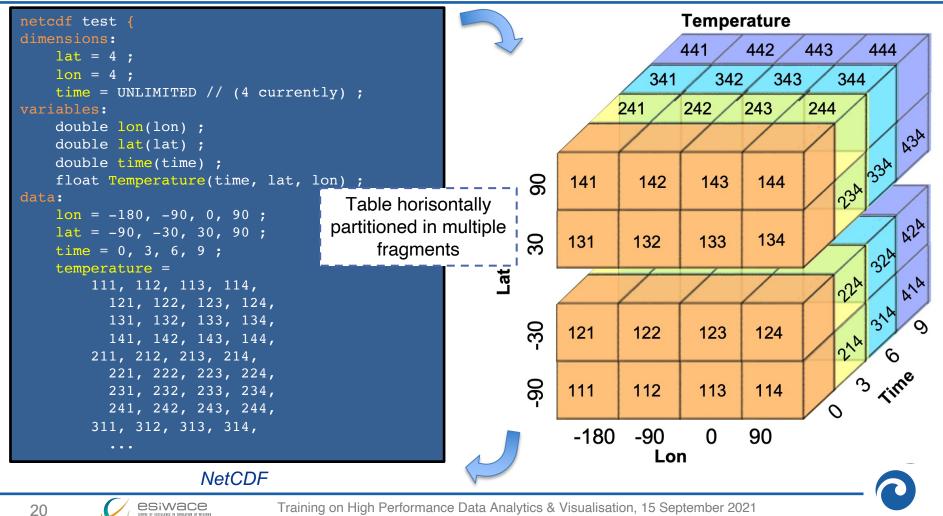
ESIWACE CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

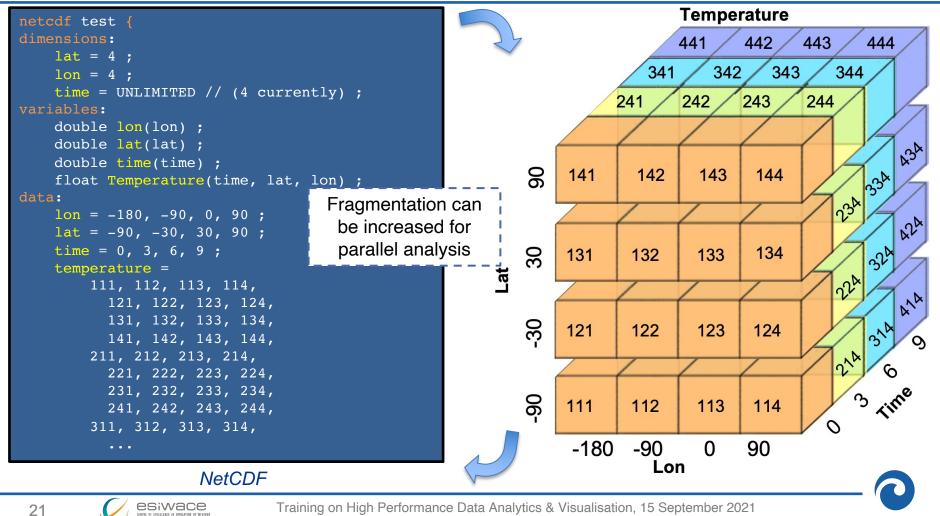
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<pre>netcdf test { dimensions:</pre>							
						erature	
lat = 4 ;		lat	lon	time[0]	time[1]	time[2]	time[3]
lon = 4;	7>	-90	-180	111	211	311	411
<pre>time = UNLIMITED // (4 current variables:</pre>	ειý) ;	-90	-90	112	212	312	412
		-90	0	113	213	313	413
<pre>double lon(lon) ; double lat(lat) ;</pre>		-90	90	114	214	314	414
double time(time);		-30	-180	121	221	321	421
float Temperature(time, lat, 1	lon) •	-30	-90	122	222	322	422
data:			0	122	223	323	423
lon = -180, -90, 0, 90;	Table horizontal	1y 20					
lat = -90, -30, 30, 90;	partitioned in multi	iple -30	90	124	224	324	424
time = 0, 3, 6, 9;	fragments	i i					
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121, 122, 123, 124, 131, 132, 133, 134, 141, 142, 143, 144,		30 30 30 30	-180 -90 0 90	131 132 133 134	time[1] 231 232 233 234	time[2] 331 332 333 334	431 432 433 434
121, 122, 123, 124, 131, 132, 133, 134, 141, 142, 143, 144, 211, 212, 213, 214,		30 30 30	-180 -90 0	131 132 133	time[1] 231 232 233	time[2] 331 332 333	431 432 433
121, 122, 123, 124, 131, 132, 133, 134, 141, 142, 143, 144, 211, 212, 213, 214, 221, 222, 223, 224,		30 30 30 30	-180 -90 0 90	131 132 133 134	time[1] 231 232 233 234	time[2] 331 332 333 334	431 432 433 434
121, 122, 123, 124, 131, 132, 133, 134, 141, 142, 143, 144, 211, 212, 213, 214, 221, 222, 223, 224, 231, 232, 233, 234,		30 30 30 30 90	-180 -90 0 90 -180	131 132 133 134 141	time[1] 231 232 233 234 241	time[2] 331 332 333 334 341	431 432 433 434 441
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,		30 30 30 30 90 90	-180 -90 0 90 -180 -90	131 132 133 134 141 142	time[1] 231 232 233 234 241 242	time[2] 331 332 333 334 341 342	431 432 433 434 441 442

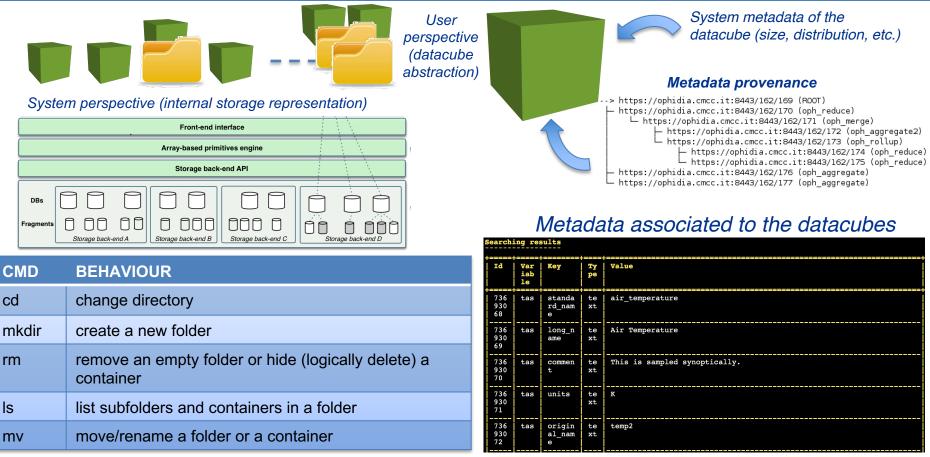


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Data abstraction: cube space perspective



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

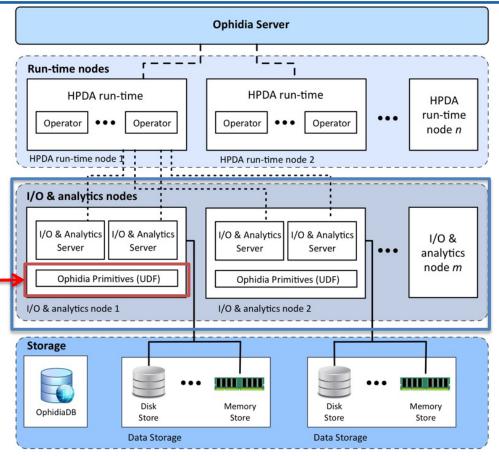
Multiple **I/O & analytics nodes** execute one or more servers

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



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 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**'))

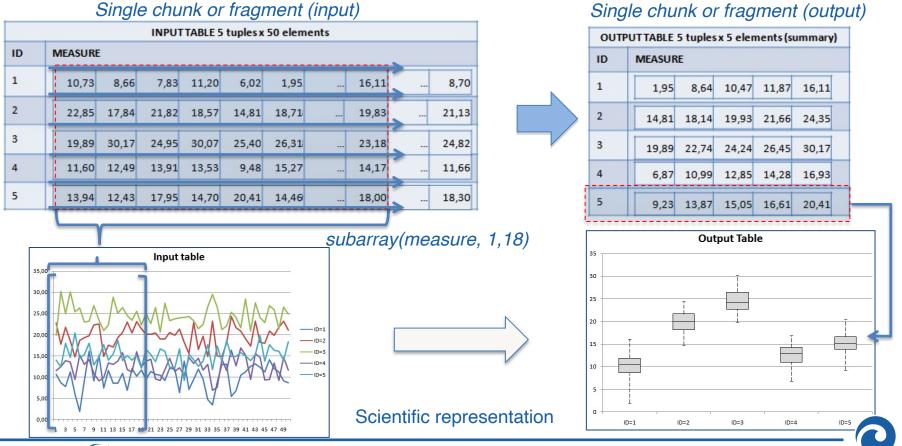
Ophidia Primitives documentation: http://ophidia.cmcc.it/documentation/users/primitives/index.html





Array-based primitives: nesting support

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



Training on High Performance Data Analytics & Visualisation, 15 September 2021

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Ophidia architecture: HPDA runtime layer

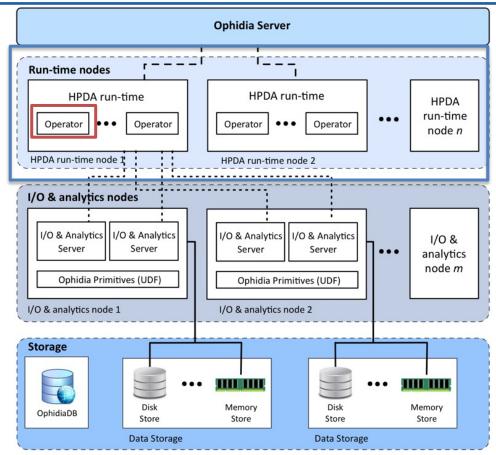
The Ophidia HPDA runtime system can be executed with *multiple processes/threads* and *distributed over multiple nodes*

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



"metadata" operators

[37..4416] >> oph_cubeio

[Request]:

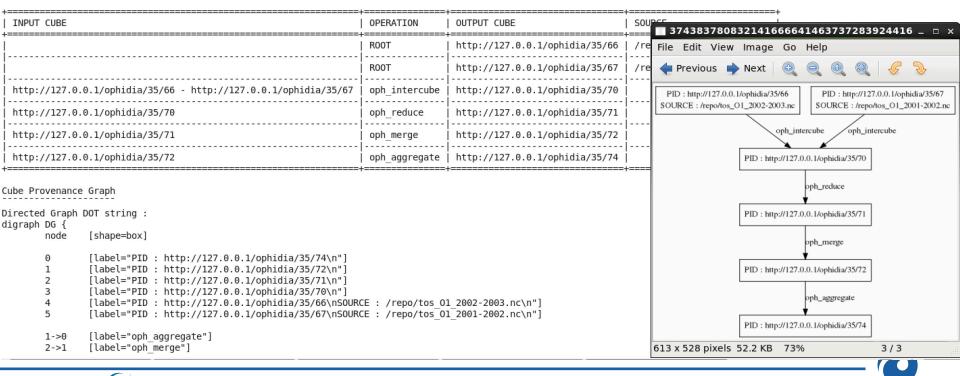
operator=oph_cubeio;sessionid=http://127.0.0.1/ophidia/sessions/374383780832141666641463737283924416/experiment;exec_mode=sync;ncores=1;cube=http://127.0.0.1/ophidia/35/74;cwd=/;

[JobID]:

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

[Response]:

Cube Provenance



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Ophidia architecture: front-end layer

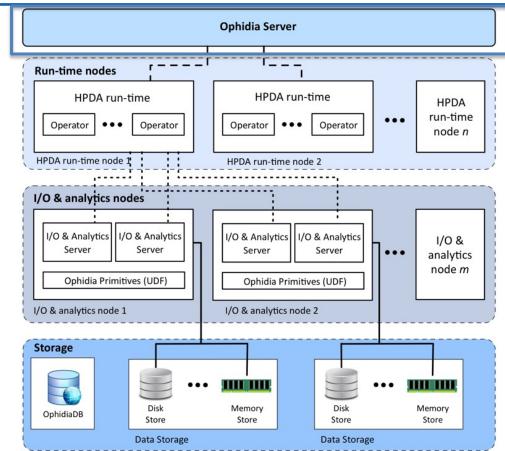
The *Ophidia Server* is the *multi-interface* server front-end

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



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;

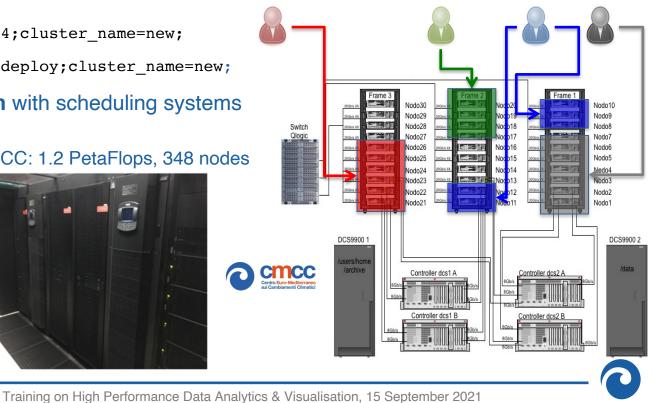
Transparent interaction with scheduling systems

Zeus SuperComputer at CMCC: 1.2 PetaFlops, 348 nodes



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

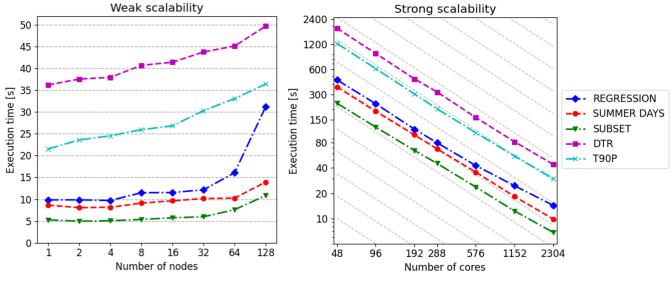


Ophidia HPDA framework benchmark

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

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).



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

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Introduction to HPDA and data challenges in eScience

Overview of the Ophidia HPDA framework

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Ophidia Python bindings: PyOphidia

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Programmatic support for data science applications

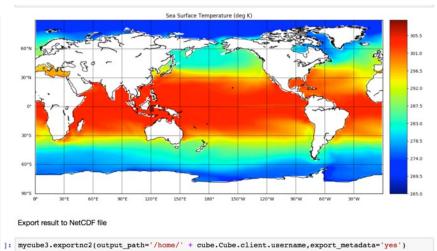
PyOphidia is a Python module to interact with the Ophidia framework.

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 ۲
- 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 jupyterhub Icing_Days (read only) Logout Control Panel jupyterhub Summer_Days (read only) Logout Control Panel Not Trusted / Ø Python 3 O Python 3 O View Insert Cell Kernel Edit View Insert Cell Kernel Widgets . . 3< 2 15 + + H Run E C H Markdown - 🖽 2 1 + + H Run = C + Code clevs = np.arange(np.nanmin(var), np.nanmax(var)+levstep, levstep) clevs = np.arange(np.nanmin(var), np.nanmax(var)+levStep, levStep) #Set filled contour plot #Set filled contour plot cnplot = ax.contourf(x, y, var_cyclic, clevs, transform=projection,cmap=plt.cm.Blues) cnplot = ax.contourf(x, y, var_cyclic, clevs, transform=projection,cmap=plt.cm.Oranges) plt.colorbar(cnplot,ax=ax) plt.colorbar(cnplot,ax=ax) ax.set_aspect('auto', adjustable=None) ax.set_aspect('auto', adjustable=None) plt.title('Icing Days') 1+ +itla("Summer Dave") plt.show() jupyterhub Daily_Temperature_Range (read only) Logout Control Panel Icing Days Summer Dave Not Trusted & 🔗 Python 3 O . . 329.4 cnplot = ax.contourf(x, y, var_cyclic, clevs, transform=projection,cmap=plt.cm.Oranges)
plt.colorbar(cnplot,ax=ax) Logout Control Panel Not Trusted & 🔗 Python 3 O ax.set_aspect('auto', adjustable=None) . . plt.title('DTR (deg K)') Code plt.show() (var), np.nanmax(var)+levStep, levStep) DTR (deg K) var cyclic, clevs, transform=projection,cmap=plt.cm,Blues) 17.03 stable-None) 14.25 ~ Frost Days 11.41 **Tropical Nights** 329.4 8.72 274.5 5.95 219.6 3.19 164.7 109.8 109.8 54.9 - 54.9

Training on High Performance Data Analytics & Visualisation, 15 September 2021

esiwace

CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER

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

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Questions?

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More about Ophidia?

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

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

Contact: ophidia-info [at] cmcc.it

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

