High Perfomance Data Analytics in eScience

Lab Tutorial

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On behalf of the ECAS Team



ESiWACE2 Summer School on Effective HPC for Climate and Weather 26 August 2020



Session outline

✓ Brief introduction to Jupyter Notebook

✓ PyOphidia modules and interface

✓ VMI environment for the Virtual Lab

✓ Overview of ECASLab @ CMCC

✓ PyOphidia notebook demo



Jupyter Notebook



"The **Jupyter** Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text. Uses include: data cleaning and transformation, numerical simulation, statistical modeling, data visualization, machine learning, and much more." ¹

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¹Jupyter Website: https://jupyter.org/



The PyOphidia library

PyOphidia is a GPLv3-licensed Python module to interact with the Ophidia framework and it implements two main classes:

- Client class: supports the submissions of Ophidia commands and workflows, as well as the management of session from Python code (similar to the Ophidia Terminal)
 - o It allows to run all the Ophidia operators, including massive tasks and workflows
- Cube class: provides the datacube type abstraction and the methods to manipulate, process and get information on cubes objects and it builds on the client class
 - Defines a object-oriented approach allowing to handle a datacube more naturally

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



PyOphidia Cube class introduces the concept of **cube objects** and supports all the Ophidia operators as **methods**.

To this end, the class defines two types of methods according to the type of operator:

 Class methods: concerning the operators which do not refer to a particular cube object (e.g. the oph_list, the operators to manage the file system, etc.)

cube.Cube.list(level=2)

 Instance methods: concern the operators applied directly on a cube object to access and manipulate it (by creating a new cube object)

```
mycube.info()
```

mycube2 = mycube.reduce(operation='max', ncores=5)



Example of **cube class** usage:

• Load the module and setup a connection to the server instance (similar to client class)

• The arguments can be automatically inferred by the environment, if setup in the .bashrc

```
cube.Cube.setclient(read_env=True)
```

 Once the connection has been setup all the operators can be executed remotely through the related method

```
cube.Cube.list(level=2)
```



Example of **cube class** usage:

• A cube object can be created in multiple ways. In case of pre-existing cube (pid):

mycube = cube.Cube(pid='http://127.0.0.1/ophidia/1/1')

• A cube can be also created from a NetCDF file using the constructor function:

mycube = cube.Cube(exp_dim='lat|lon', imp_dim='time', ncores=2 measure='tos', src_path='/path/tos.nc')

o or directly using the import method (exactly the same as the previous one):

mycube = cube.Cube.importnc(exp_dim='lat|lon',imp_dim='time',ncores=2 measure='tos',src_path='/path/tos.nc')

• After the processing, the cube can be deleted with the proper method:

mycube.delete()



Example of **cube class** usage:

 Once a cube is available in the python code, various operators can be executed to produce new datacubes:

```
mycube2 = mycube.reduce(operation='max', ncores=5)
```

```
mycube4 = mycube3.aggregate(operation='max', ncores=5)
```

Methods can also be concatenated into a single command:



The client class allows to run the same commands of the cube class with a lowerlevel interface and supports the execution of massive operators (param. sweep)

o Commands follow the same structure as for the Oph_term (oph_operator param1=val1;)

```
from PyOphidia import client
ophclient = client.Client(read env=True)
```

ophclient.submit("oph_list level=1", display=True)

• Multiple files can be loaded in parallel by specifying a filter on the inputs

ophclient.submit("oph_importnc exp_dim=lat|lon;imp_dim=time;ncores=2; measure=tos;src_path=[path=/path/*.nc]")

o The same operator can be run in parallel on multiple input cubes

ophclient.submit("oph_reduce2 operation=avg;dim=time;cube=[*]")

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



Virtual Lab environment

The pre-installed VMI with the full Ophidia stack and other dependencies for the Virtual Lab is available at: <u>https://download.ophidia.cmcc.it/vmi_desktop/training/OphidiaVMI.ova</u>

Login and password are both **ophidia**. For additional information refer to the summer school virtual lab instructions.





ECASLab @ CMCC



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ECASLab is a scientific data analytics environment built on top of ECAS (the ENES Climate Analytics Service), one of the thematic services included in the EOSC-hub service portfolio.

It provides a scientific environment exploiting a server-side approach and integrating both data and analysis tools to support data scientists in their daily research activities.

ECASLab starts from a previous effort (OphidiaLab, developed at CMCC Foundation) with the main aim of providing a virtualized research environment for researchers. It represents the entry point for users that want to test, train, exploit the ECAS Thematic Service.



A few examples of output related to different analytics experiments implemented in the ECASLab environment.

It consists of several components like an ECAS cluster, a JupyterHub instance jointly with a large set of pre-installed Python libraries for running data manipulation, analysis, and visualization, a data publication service and a tool for the infrastructure monitoring (mainly intended for the administrators).

In order to get started with ECASLab please have a look at the Quick Start section and register here to get an account.

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https://ecaslab.cmcc.it/

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ECASLab Registration form @CMCC



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ECASLab Registration Form

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Select IS-ENES3 as project	Affiliation *	Specify motivation
	Country *	for requesting access. You can
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ECASLab JupyterHub service

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PyOphidia notebook demo: ECAS_Basics

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	First of all import PyOphidia modules and connect to server (connection details are inferred from	n the EC	CAS enviro	onmei	nt)
In []:	<pre>from PyOphidia import cube, client cube.Cube.setclient(read_env=True)</pre>				
	Create a datacube from the NetCDF file:				
	The file is data/ecas_training/tasmax_day_CMCC-CESM_rcp85_r1i1p1_20960101-2100	1231.nd	•		
	 The variable to be imported is tasmax Data should be arranged in order to operate on time series (time dimension) 				
	Note: we are not directly reading the me from the Notebook				
In []:	<pre>mycube = cube.Cube.importnc(</pre>	i rlilı	51 20960	101-	-2100123
	measure='tos',				
	<pre>imp_dim='time', ioserver='ophidiaio_memory',</pre>				
	ncores=2,				
)				
	Check the datacubes available in the virtual file system				



Links and references

Virtual Lab

- Ophidia Virtual Machine Image: <u>https://download.ophidia.cmcc.it/vmi_desktop/training/OphidiaVMI.ova</u>
- Updated training material: <u>https://github.com/ECAS-Lab/ecas-training/tree/ESiWACE2_SummerSchool_2020</u> *Ophidia*
- Ophidia Website: http://ophidia.cmcc.it
- Ophidia Doc: <u>http://ophidia.cmcc.it/documentation</u>
 ECASLab
- CMCC ECASLab instance: <u>https://ecaslab.cmcc.it/</u>
- ECASLab registration form @ CMCC: <u>https://ecaslab.cmcc.it/web/registration.php</u>

PyOphidia

- PyOphidia Doc: http://ophidia.cmcc.it/documentation/users/pyophidia/
- PyOphidia repository: <u>https://github.com/OphidiaBigData/PyOphidia</u>

Other software/Python modules used in the examples

- Jupyter Project Doc: <u>https://jupyter.readthedocs.io/en/latest/</u>
- Cartopy Doc: <u>https://scitools.org.uk/cartopy/docs/latest/</u>
- Matplotlib User's Guides: <u>https://matplotlib.org/users/index.html</u>



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EOSC-hub



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