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Notebooks for documenting work-flows

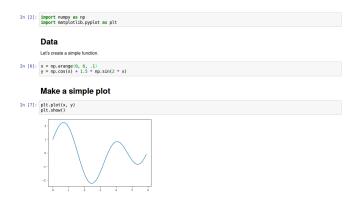
Motivation

Reproducibility

Notebooks: interactive computational environments

Notebooks combine:

- code fragments that can be executed,
- text for the description of the application and
- 3 figures illustrating the data or the results.



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"Digital Playground"

"Data Story Telling"

"Computational Narratives"

Notebooks: interactive computational environments

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- 1 code fragments that can be executed,
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```
"Interactive notebooks: Sharing the code", Nature (2014) http://www.nature.com/news/interactive-notebooks-sharing-the-code-1.16261
```

Interactive environments:

what exists today?

R-Markdown

http://rmarkdown.rstudio.com/



R-Markdown

```
http://rmarkdown.rstudio.com/
```

Creation of dynamic, self-contained documents with embedded chunks of code.

Features of interest:

- Possible to export in journal (https://github.com/rstudio/rticles) or presentation formats
- ► LATEX templates to ensure journal standards

Apache Zeppelin

https://zeppelin.apache.org/



TECHNOLOGIES







Apache Zeppelin

```
https://zeppelin.apache.org/
```

Web-based notebook for data-driven, interactive and collaborative documents. Intended for *big data* and large scale projects.

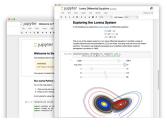
Features of interest:

- Languages can be mixed in the same notebook
- Users can to write their own interpreter (language backend)

Jupyter

http://jupyter.org/

(stands for Julia - Python - R)





The Jupyter Notebook

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



Language of choice



Share notebooks



Interactive widgets



Big data integration

Jupyter

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http://jupyter.org/ (stands for Julia - Python - R)
```

Web application for the creation and sharing of notebook-type documents.

Evolved from IPython, a command shell for interactive computing (2001).

Features of interest:

- ► More than 40 language *kernels* available
- Can be used as a multi-user server (jupyterhub)
 - ightarrow avoid installation steps on several users' machine

Beaker

http://beakernotebook.com/



The Perfect Tool for Iterative Exploration

Beaker

http://beakernotebook.com/

Notebook-style development environment for working interactively with large and complex datasets.

Features of interest:

- Usage of different languages in different cells, within the same notebook
- Language manager

CoCalc

https://cocalc.com/

"Collaborative Calculation in the Cloud"



Policies Pricing API Run CoCalc



Online computing environment

CoCalc

```
https://cocalc.com/
```

"Collaborative Calculation in the Cloud"

Web-based cloud computing platform, formerly called formerly called SageMathCloud.

Features of interest:

- Support of many languages
- Users to upload their file on the platform to be later read or processed

|--|

Tool name	R- Markdown	jupyter	beaker	Cocalc	Zeppelin
GitHub	rmarkdown	notebook	beakerx	cocalc	zeppelin

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GitHub	rmarkdown	notebook	beakerx	cocalc	zeppelin
Languages	R, Python, SQL, Bash, Rcpp, Stan, JavaScript	Julia, Python, R, Scala, Bash, Octave, Rubi, Fortran, PHP,	Julia, Python, R, Javascript, C++, Torch, Scala, Bash, Octave, Rubi, Fortran,	R, Python, Octave, Cython, Julia, Java, C/C++, Perl, Ruby	Scala, Python, SparkSQL, Hive, Markdown

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Export formats	HTML, PDF, MS Word, Beamer, HTML5 slides,	PDF, LaTeX, HMTL, Markdown, reST	Beaker format		JSON

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Cloud deployment	-	JupyterHub	Beaker Lab (discontinued)	-	Yes

Summary

- Most of the environments provides supports for many languages
- 2 Beaker is the only option allowing the mix of different languages but its installation/utilisation are not trivial
- JupyterHub is an option for the deployment on a server so that multiple users can work at the same time using the same infrastructure

Notebook example:

divaND interpolation

A quick example of how to document workflow

Click here

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- Notebooks are not Virtual Research Environment, but can be one of their components
- 3 Notebooks are not new (15 years) but their use has evolved
- 4 Such a tool is great to document a workflow Example: climatology production

Future work

Examples using SeaDataCloud data

Future work

- 1 Examples using SeaDataCloud data
- 2 Application with data API

(SOCIB, OneStop)

Future work

- Examples using SeaDataCloud data
- 2 Application with data API
- 3 Notebook citation

(SOCIB, OneStop)
See on Wednesday