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# *Notebooks for documenting work-flows*

# Motivation

Reproducibility

# Notebooks: interactive computational environments

*Notebooks* combine:

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

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
```

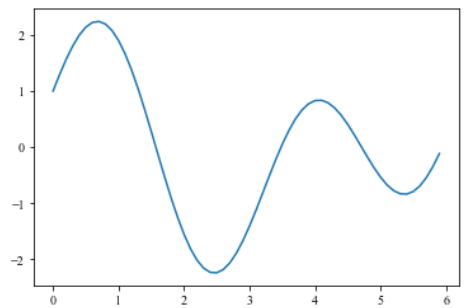
### Data

Let's create a simple function.

In [6]:
```
x = np.arange(0, 6, .1)
y = np.cos(x) + 1.5 * np.sin(2 * x)
```

### Make a simple plot

In [7]:
```
plt.plot(x, y)
plt.show()
```



# Notebooks: interactive computational environments

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*"Digital Playground"*

*"Data Story Telling"*

*"Computational Narratives"*

# Notebooks: interactive computational environments

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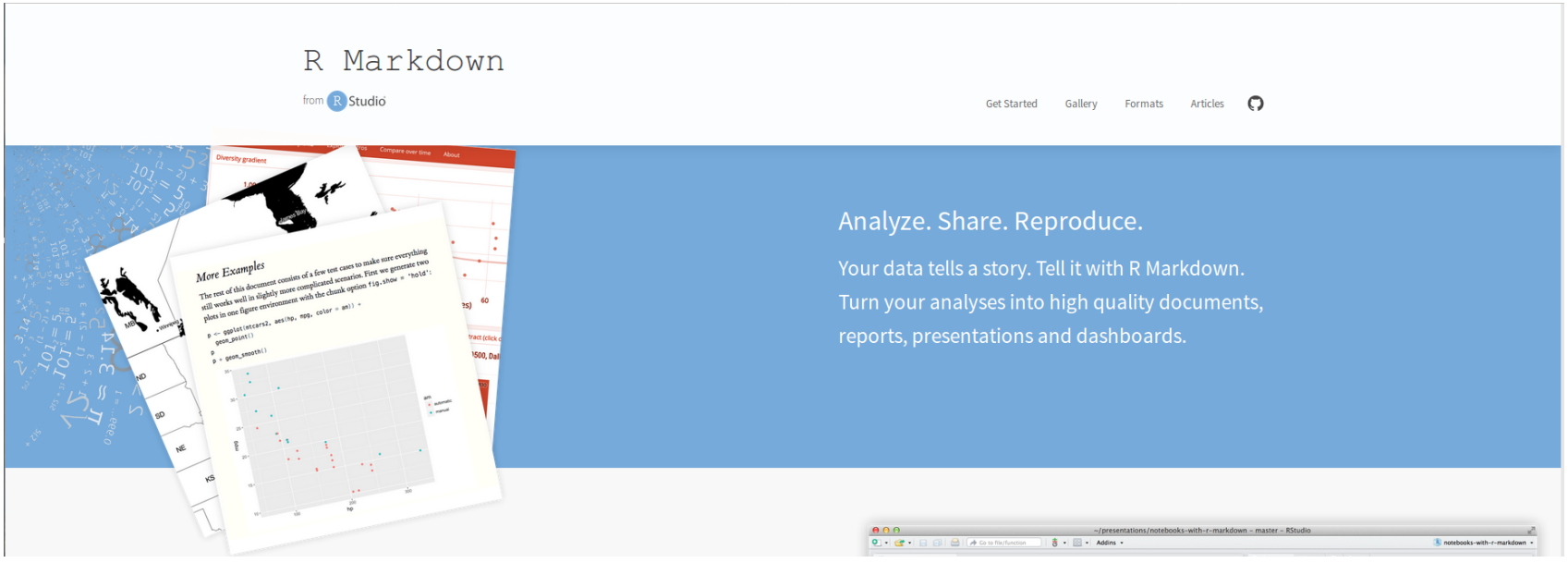
"Interactive notebooks: Sharing the code", Nature (2014)
http://www.nature.com/news/interactive-notebooks-sharing-the-code-1.16261

# *Interactive environments:*

what exists today?

# R-Markdown

http://rmarkdown.rstudio.com/



# R-Markdown

http://rmarkdown.rstudio.com/

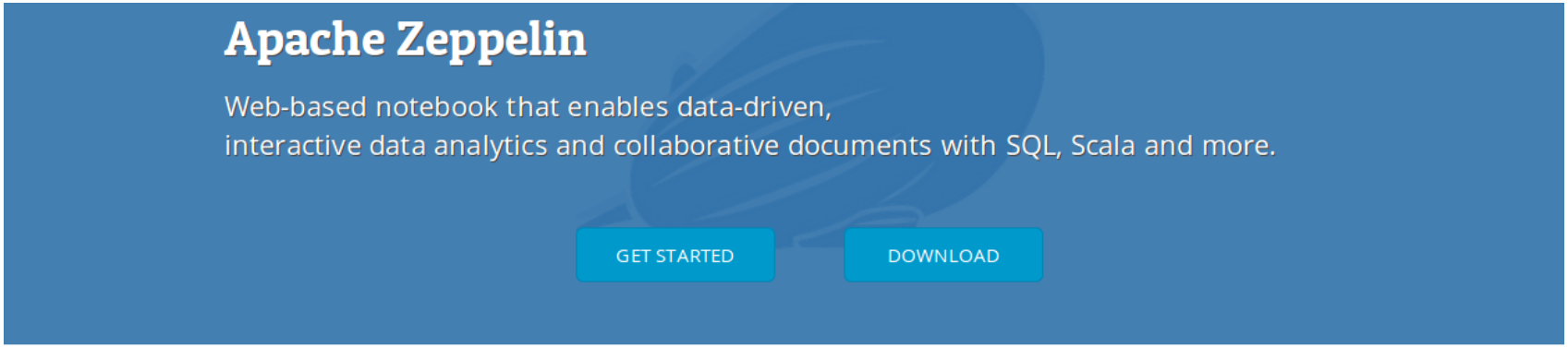
Creation of dynamic, self-contained documents with embedded chunks of code.

Features of interest:

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

# Apache Zeppelin

https://zeppelin.apache.org/




TECHNOLOGIES

Apache Spark | SQL | python

# Apache Zeppelin

https://zeppelin.apache.org/

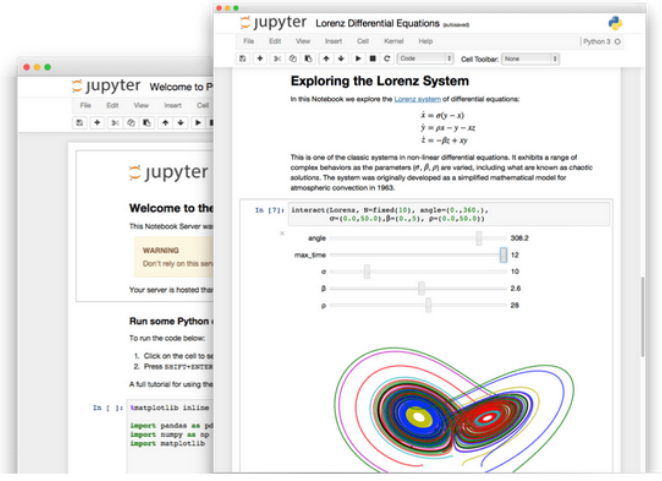
Web-based notebook for
data-driven, interactive and collaborative documents.
Intended for *big data* and large scale projects.

Features of interest:

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

# Jupyter

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




## The 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 explanatory text. Uses include: data cleaning and transformation, numerical simulation, statistical modeling, machine learning and much more.

</> Language of choice

Share notebooks

Interactive widgets

Spark Big data integration

# Jupyter

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

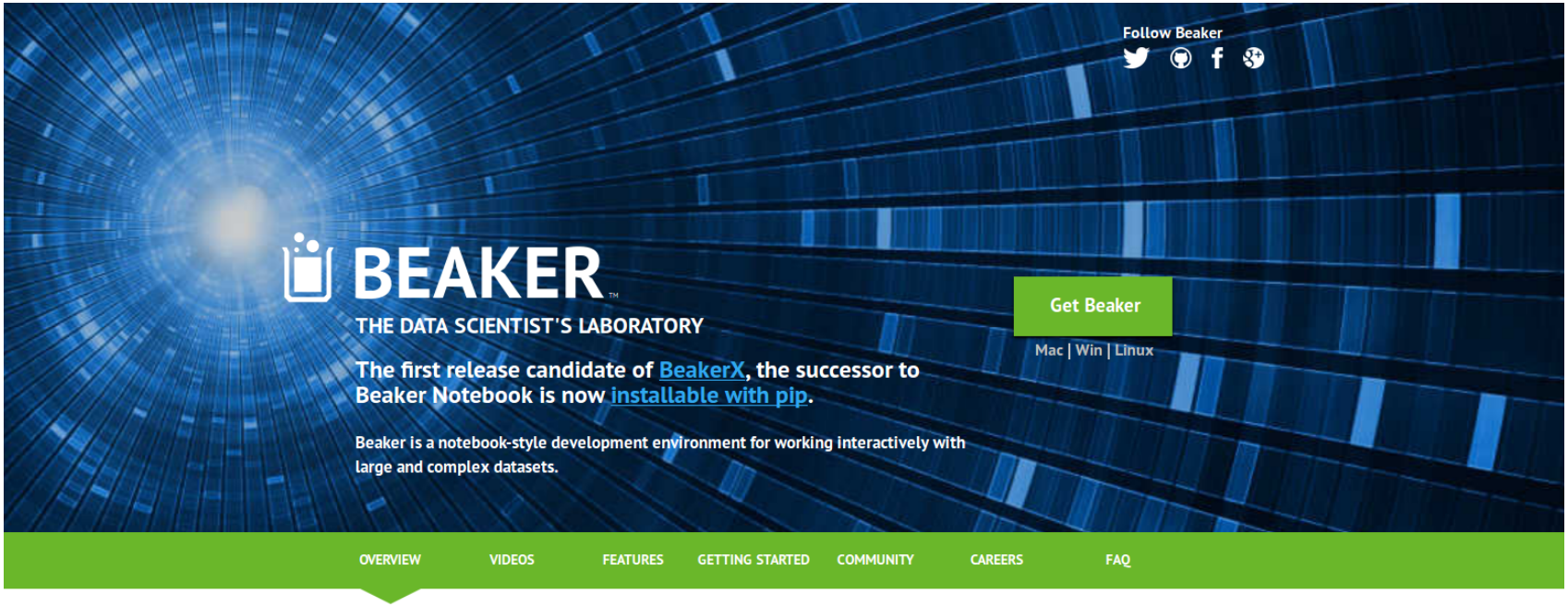
Web application for the creation and sharing of notebook-type documents.
Evolved from IPython, a command shell for interactive computing (2001).

Features of interest:

- More than 40 language *kernels* available
- Can be used as a multi-user server (`jupyterhub`)
  $\rightarrow$ 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*"


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

# Comparison

| **Tool name** | R-Markdown | jupyter | beaker | 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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| **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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| **Cloud deployment** | – | JupyterHub | Beaker Lab (discontinued) | – | Yes |

# Summary

1. 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
3. 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

# Conclusions

1. Notebooks are interactive computational environments combining code, text, results, figures...

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3. Notebooks are not new (15 years) but their use has evolved

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1. Notebooks are interactive computational environments combining code, text, results, figures...
2. 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

1. Examples using SeaDataCloud data

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2. Application with data API (SOCIB, NOAA OneStop)

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1. Examples using SeaDataCloud data
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3. Notebook citation See on Wednesday