

IPython: modern tools for interactive & web-enabled scientific computing

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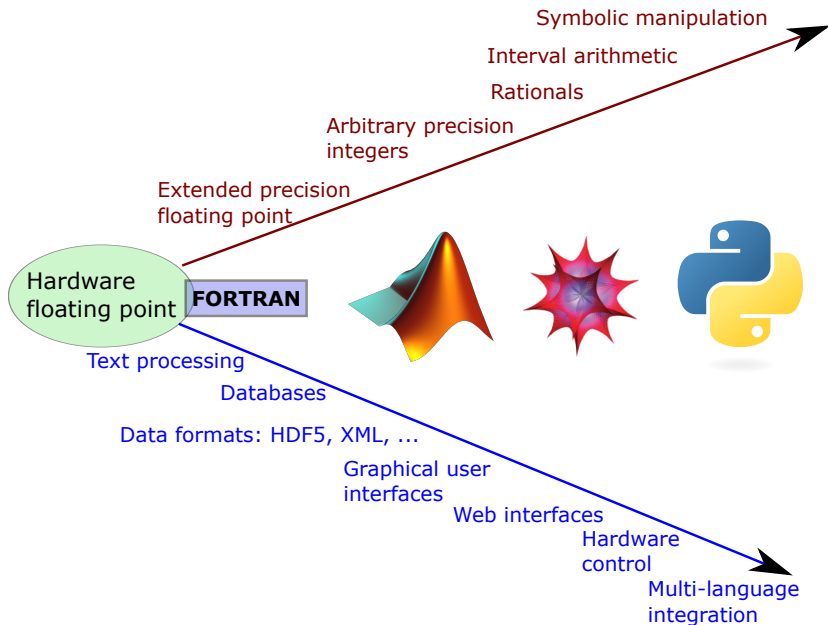
NERSC User Day, LBL, Berkeley,
Feb 13, 2013

Outline

1 Scientific Python

2 IPython: Interactive Python

Beyond (Floating Point) Number Crunching



Scientific Python: a Rich Ecosystem



IPython



Outline

1 Scientific Python

2 IPython: Interactive Python

The Lifecycle of a Scientific Idea (schematically)

- 1 Individual exploratory work
- 2 Collaborative development
- 3 Production work (HPC, cloud, parallel)
- 4 Publication (with reproducible results!)
- 5 Education
- 6 Goto 1.

The Problem with most tools

Barriers and discontinuities in workflow in between all the steps

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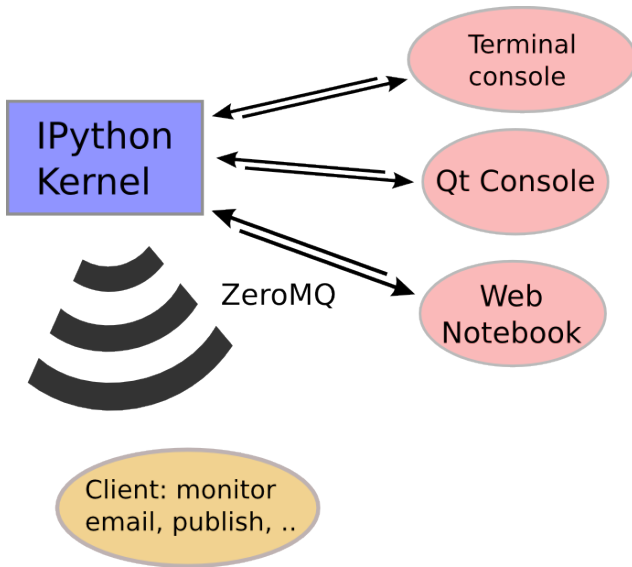
The Problem with most tools

Barriers and discontinuities in workflow in between all the steps

IPython's goal:
Fluid transitions in all these steps

Demo

Pillar #1: An architecture for interactive computing



Pillar #2: the Notebook Format

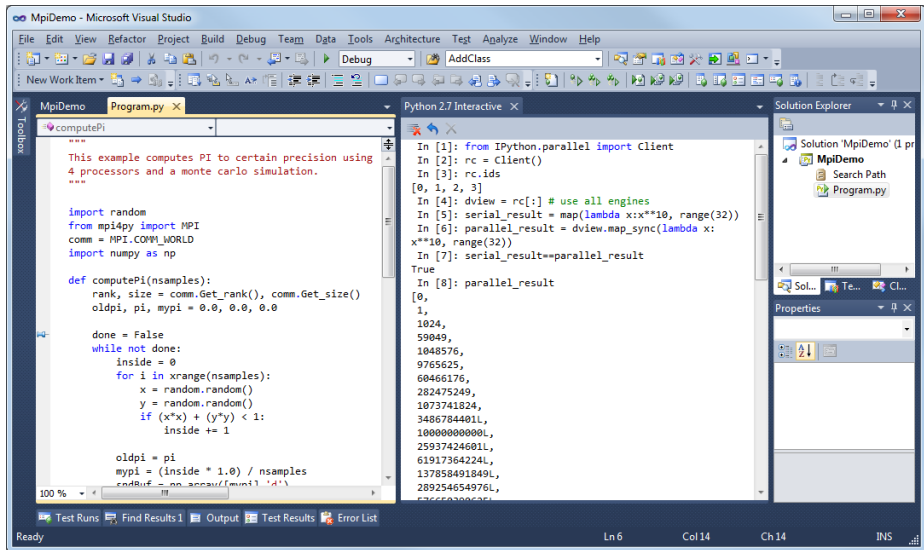
- **JSON** but version control-friendly
- Easy for machine processing, **fixable by hand if need be**.
- Lots of hooks for **metadata**
- **Not Python-specific** (R and Ruby notebooks exist, Julia planned)
- Produce Markdown, reST, $\text{\LaTeX}$, HTML, etc...

An open format for **sharing, publishing and archiving** executable computational work

Documented protocols and formats: a growing ecosystem around IPython

Microsoft Visual Studio 2010 integrated console

Dino Viehland and Shahrokh Mortazavi (Microsoft); <http://pytools.codeplex.com>



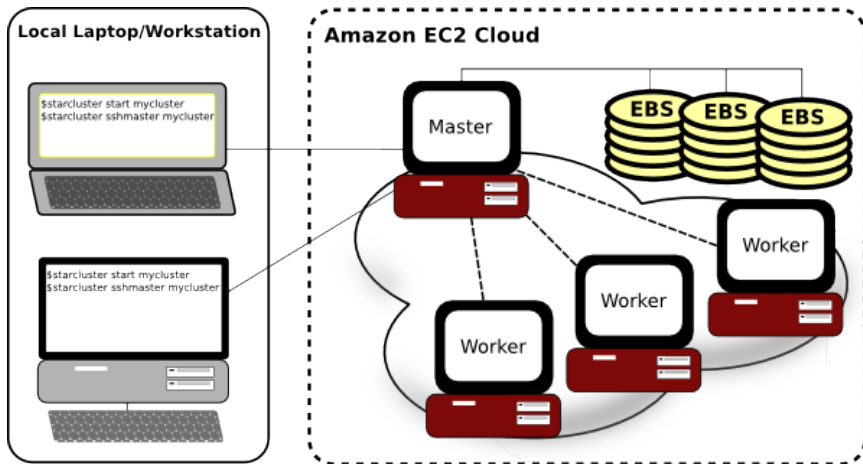
Notebooks on Windows Azure Cloud

Shahrokh Mortazavi (Microsoft), B.G., F.P.: <http://bit.ly/JQeoJD>.

The screenshot displays the Windows Azure website's 'Python - IPython Notebook' tutorial page. The browser's address bar shows the URL <https://www.windowsazure.com/en-us/develop/python/tutorials/ipython-notebook/>. The page features a navigation bar with links for HOME, PRICING, DEVELOP, MANAGE, COMMUNITY, SUPPORT, and ACCOUNT. Below this, a secondary navigation bar lists 'overview', '.net', 'node.js', 'php', 'java', 'python', and 'downloads'. A 'Free trial' button is visible in the top right corner. The main content area is titled 'IPython Notebook on Windows Azure' and includes a play button icon. The left sidebar contains sections for 'WINDOWS AZURE INTRO', 'TUTORIALS' (with links to Web with Django, Web with Django + MySQL, and Django with Visual Studio), 'IPython Notebook' (with a 'show all' link), 'HOW TO GUIDES' (listing various services like Blob Service, Table Service, Queue Service, etc.), 'COMMON TASKS' (listing tasks like Install Python, SQL Database Management, etc.), and 'BEST PRACTICES' (listing Troubleshooting, Security, etc.). An inset image at the bottom right shows a screenshot of the IPython Notebook interface, displaying a 'spectrogram' notebook with a menu bar (File, Edit, View, Insert, Cell, Kernel, Help) and a toolbar. The notebook title is 'IPython Notebook spectrogram' and it shows 'Last saved: Feb 23 5:19 PM'. The content area of the notebook shows the text 'Simple spectral analysis'.

Star Cluster: IPython parallel+Notebook on Amazon EC2

Justin Riley (MIT): <http://web.mit.edu/star/cluster>



One-click single notebook on Amazon EC2

Carl Smith (UK): <https://notebookcloud.appspot.com>.

The screenshot shows a web browser window with the title 'NotebookCloud'. The address bar displays 'https://notebookcloud.appspot.com'. Below the address bar is a navigation bar with links: 'NBCloud Docs', 'IPython Docs', 'Account Details', and 'Delete Account'. The user's email 'fdo.perez@gmail.com' is visible in the top right corner of the page.

The main content area is titled 'Instance Launcher'. It contains a grid of buttons for selecting instance types:

- Micro
- Small
- Medium
- Large
- XLarge

Below these, there is a section for memory and CPU options:

- High Memory
- High Memory x 2
- High Memory x 4
- High CPU Medium
- High CPU XLarge

At the bottom of the instance selection grid, there are four buttons:

- GPU Cluster
- Super Cluster
- Death Star
- Hello World

To the right of the buttons, there is text explaining the selection process:

Instance Launcher

Select any instance type to see more information about it. If you are unsure about your options, please consult the documentation.

If you are using NotebookCloud for learning programming, you should select Hello World.

Below the instance launcher section, there is a section titled 'Your NotebookCloud Servers'. It contains the text: 'No instances (launched from your NotebookCloud account) exist on your AWS account.'

At the bottom of the page, there is a footer with links: 'AWS Website', 'IPython Website', 'Python Website', and 'Carl Smith'.

Other projects using IPython

Scientific

- **Software Carpentry**
- **EPD:** Enthought Python Distribution.
- **Continuum:** Anaconda, Wakari.
- **Sage:** open source mathematics.
- **PyRAF:** Space Telescope Science Institute
- **CASA:** Nat. Radio Astronomy Observatory
- **Ganga:** CERN
- **PyMAD:** neutron spectrom., Laue Langevin
- **Sardana:** European Synchrotron Radiation
- **ASCEND:** eng. modeling (Carnegie Mellon).
- **JModelica:** dynamical systems.
- **DASH:** Denver Aerosol Sources and Health.
- **Trilinos:** Sandia National Lab.
- **DoD:** baseline configuration.
- **Mayavi:** 3d visualization, Enthought.
- **NiPy:** computational pipelines, MIT.

Web/Other

- **Visual Studio 2010:** MS.
- **Django.**
- **Turbo Gears.**
- **Pylons** web framework
- **Zope** and **Plone** CMS.
- Axon Shell, BBC
Kamaelia.
- **Schevo** database.
- **Pitz:** distributed task/bug tracking.
- **iVR** (interactive Virtual Reality).
- **Movable Python** (portable Python environment).
- ...

(Incomplete) Cast of Characters

- **Brian Granger** - Physics, Cal State San Luis Obispo
- **Min Ragan-Kelley** - Nuclear Engineering, UC Berkeley
- **Matthias Bussonnier** - Physics, Institut Curie, Paris
- **Brad Froehle** - Mathematics, UC Berkeley
- **Paul Ivanov** - Neuroscience, UC Berkeley.
- **Robert Kern** - Enthought
- **Thomas Kluyver** - Biology, U. Sheffield
- **Jonathan March** - Enthought
- **Evan Patterson** - Physics, Caltech/Enthought
- **Jörgen Stenarson** - Elect. Engineering, Sweden.
- John Hunter - TradeLink Securities, Chicago.
- Stefan van der Walt - Applied Math, U. Stellenbosch
- Prabhu Ramachandran - Aerospace Engineering, IIT Bombay.
- Satra Ghosh - MIT Neuroscience
- Gaël Varoquaux - Neurospin (Orsay, France)
- Ville Vainio - CS, Tampere University of Technology, Finland
- Barry Wark - Neuroscience, U. Washington.
- Ondrej Certik - Physics, U Nevada Reno
- Darren Dale - Cornell
- Justin Riley - MIT
- Mark Voorhies - UC San Francisco
- Nicholas Rougier - INRIA Nancy Grand Est
- Thomas Spura - Fedora project
- **Many more! (~150 commit authors)**

- **Enthought**, Austin, TX: **Lots!**
- **Microsoft**: WinHPC support, Visual Studio integration, Azure (thanks to [Shahrokh Mortazavi](#)).
- **DoD/DRC Inc**: funding through Sept. 2012 (thanks to [Jose Unpingco](#) and [Chris Kees](#)).
- **NIH**: via NiPy grant
- **NSF**: via Sage compmath grant
- **Google**: summer of code 2005, 2010.
- **Tech-X** Corp., Boulder, CO: Parallel/notebook (previous versions)



ALFRED P. SLOAN FOUNDATION

2-year funding, core team (7 people)

SIMONS FOUNDATION

**Stanford: reproducibility & data sharing
(neuroimaging, other data-intensive cases)**

- Support the development of multiple projects.
- Community-created and driven.
- A neutral ground for industry, academia and government to support scientific open source.
- 501(c)3 - donations are tax-exempt in the USA

