Agenda

1. New features available in JupyterLab and JupyterHub
2. Supercomputing with Julia

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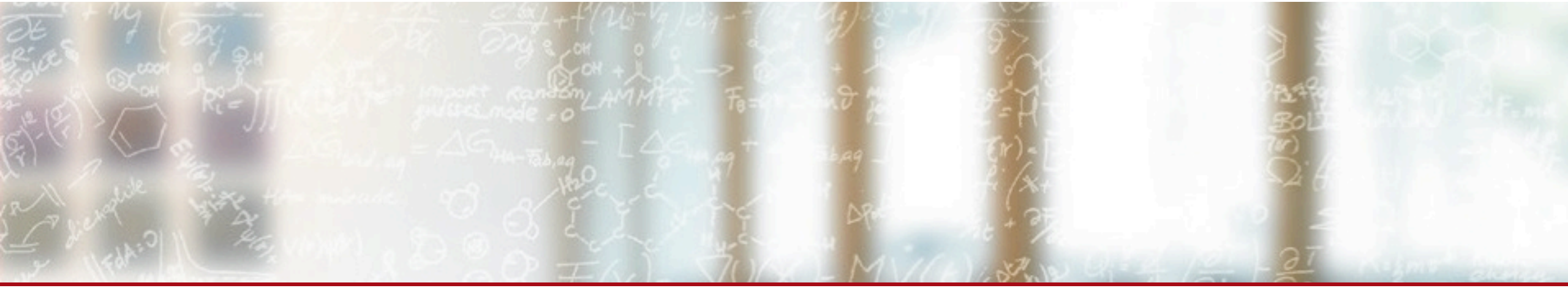


Interactive Supercomputing with Jupyter
Announcing JupyterLab 1.1.1 and JupyterHub 1.0

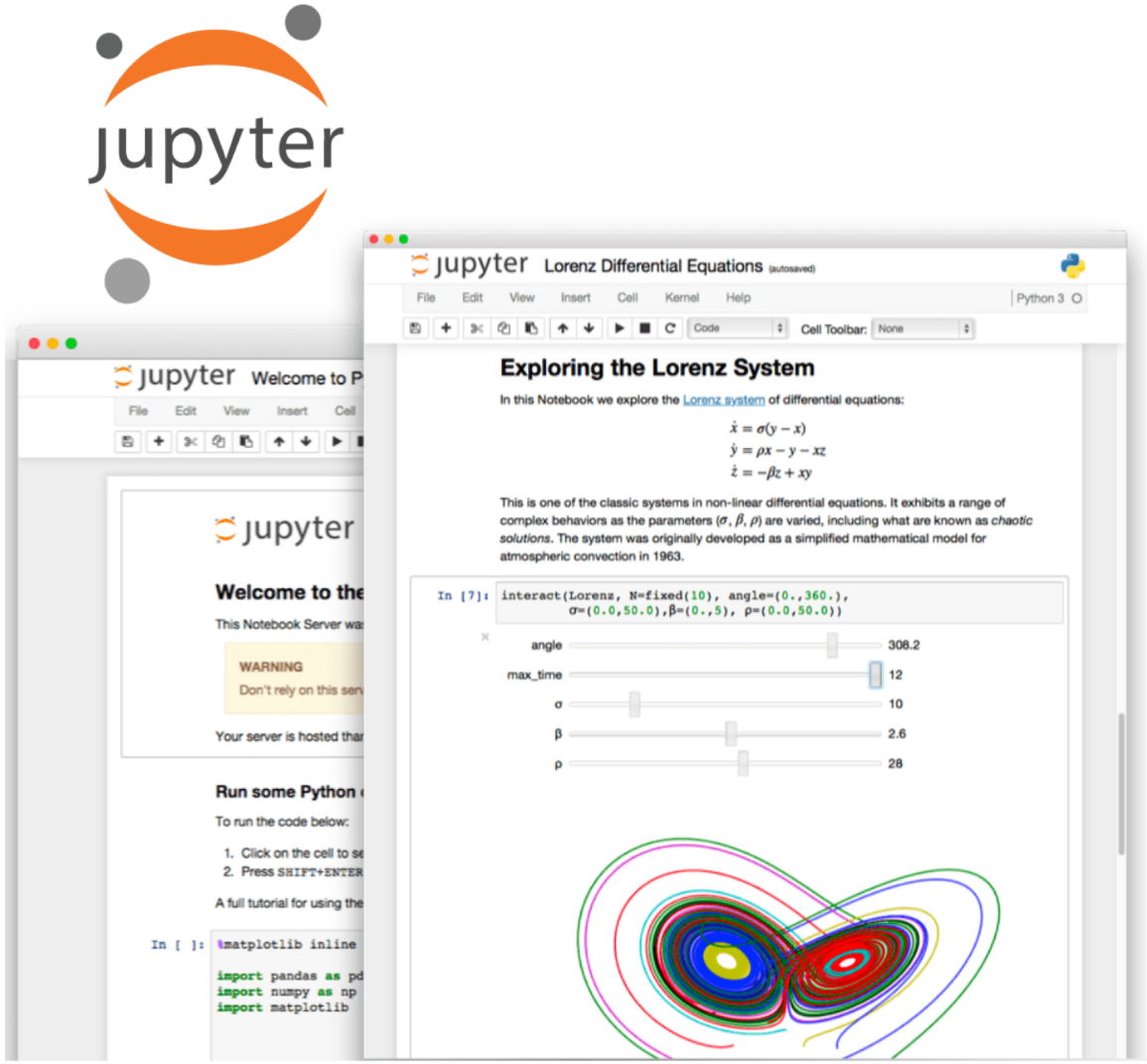
CSCS User Lab Day

Tim Robinson (ETH Zurich / CSCS)

September 9, 2019

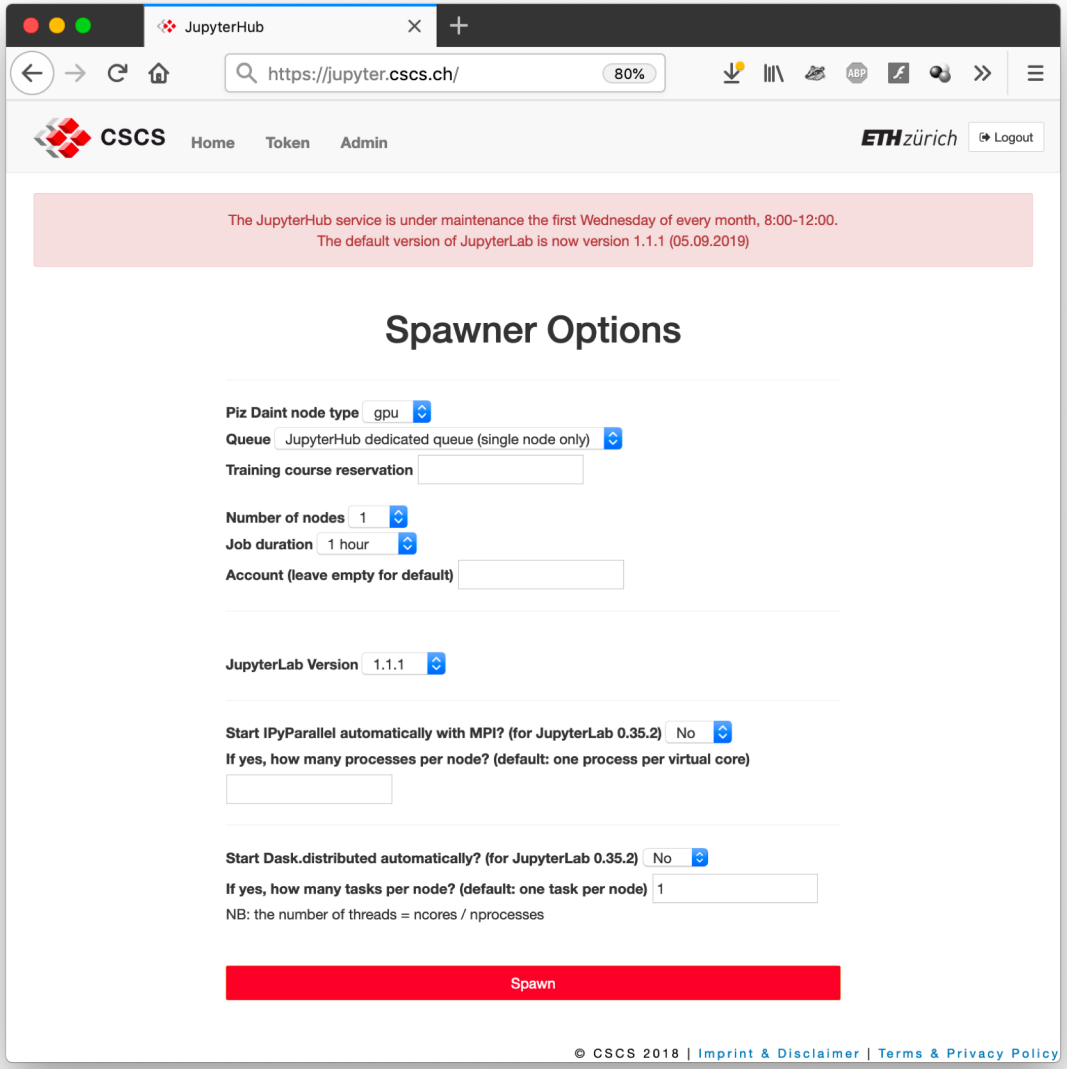
Introduction to Jupyter Notebook

- Jupyter Notebook is an open-source web app for creating reproducible computational narratives
- Documents can contain live code, equations, narrative text, visualizations, rich media, etc..
- Documents can be shared or exported to PDF, HTML, LaTeX, etc.
- Working environment includes
  - File browser
  - Terminal
  - Support for many languages: Python, R, Julia, C++, …
  - Extensible design
  - Many server/client plugins
- Notebook is attached to a “kernel”, which does the actual computation



JupyterHub for the User Lab

- **https://jupyter.cscs.ch**
- JupyterHub provides Jupyter servers on demand for users of Piz Daint
- Log in with your CSCS credentials
- Spawns a server on a dedicated compute node of Piz Daint (gpu or mc)
- Launch time should be 5 minutes maximum
- To load modules or activate virtual environments, add these commands to `$HOME/.jupyterhub.env`



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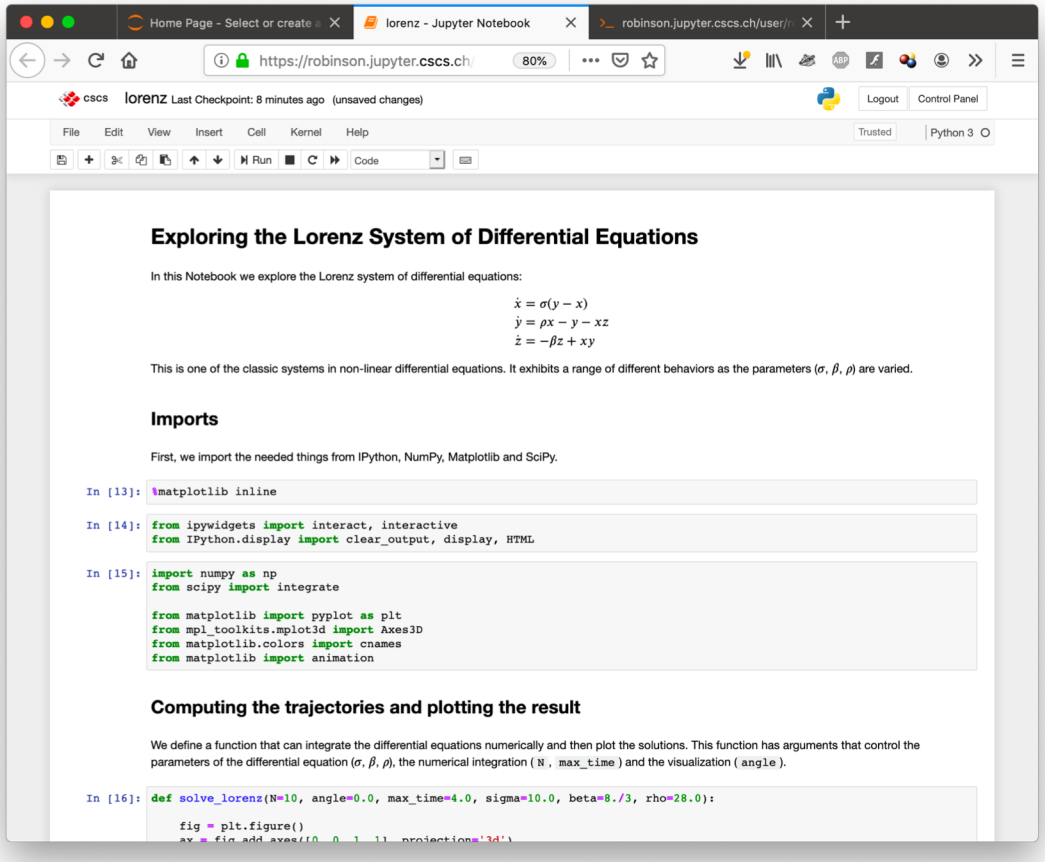
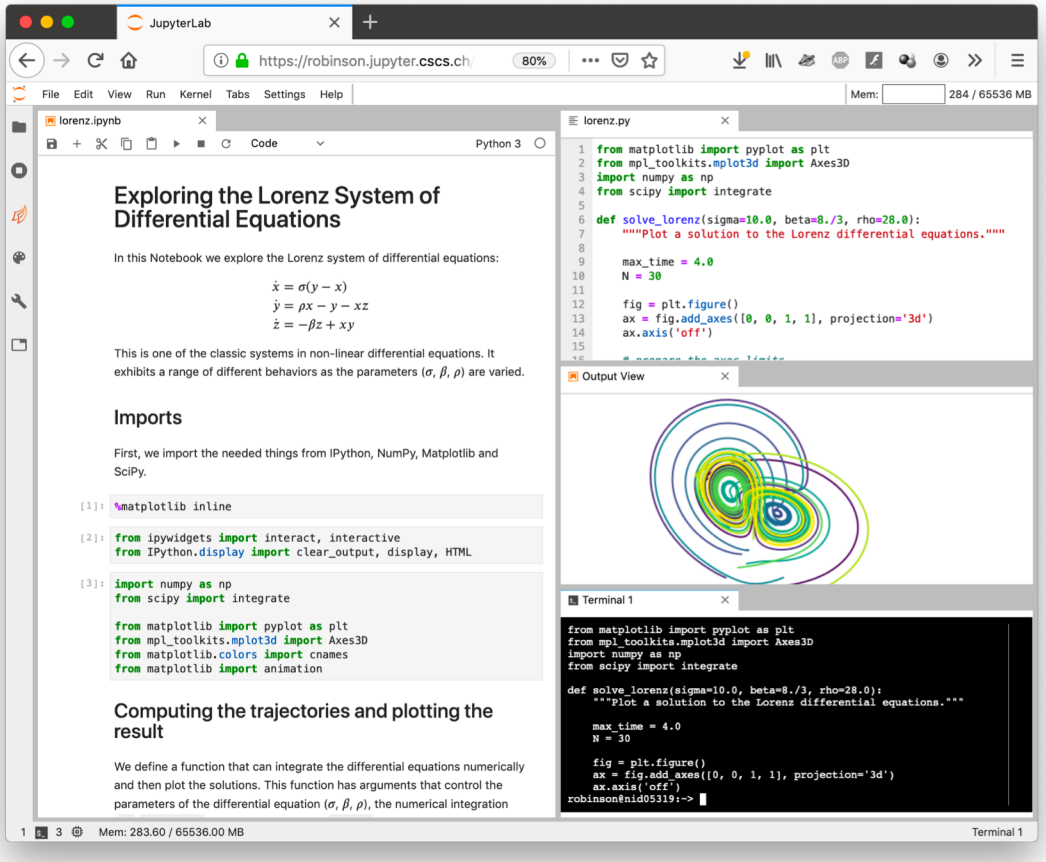
Evolution from Jupyter Notebook to JupyterLab

JupyterLab

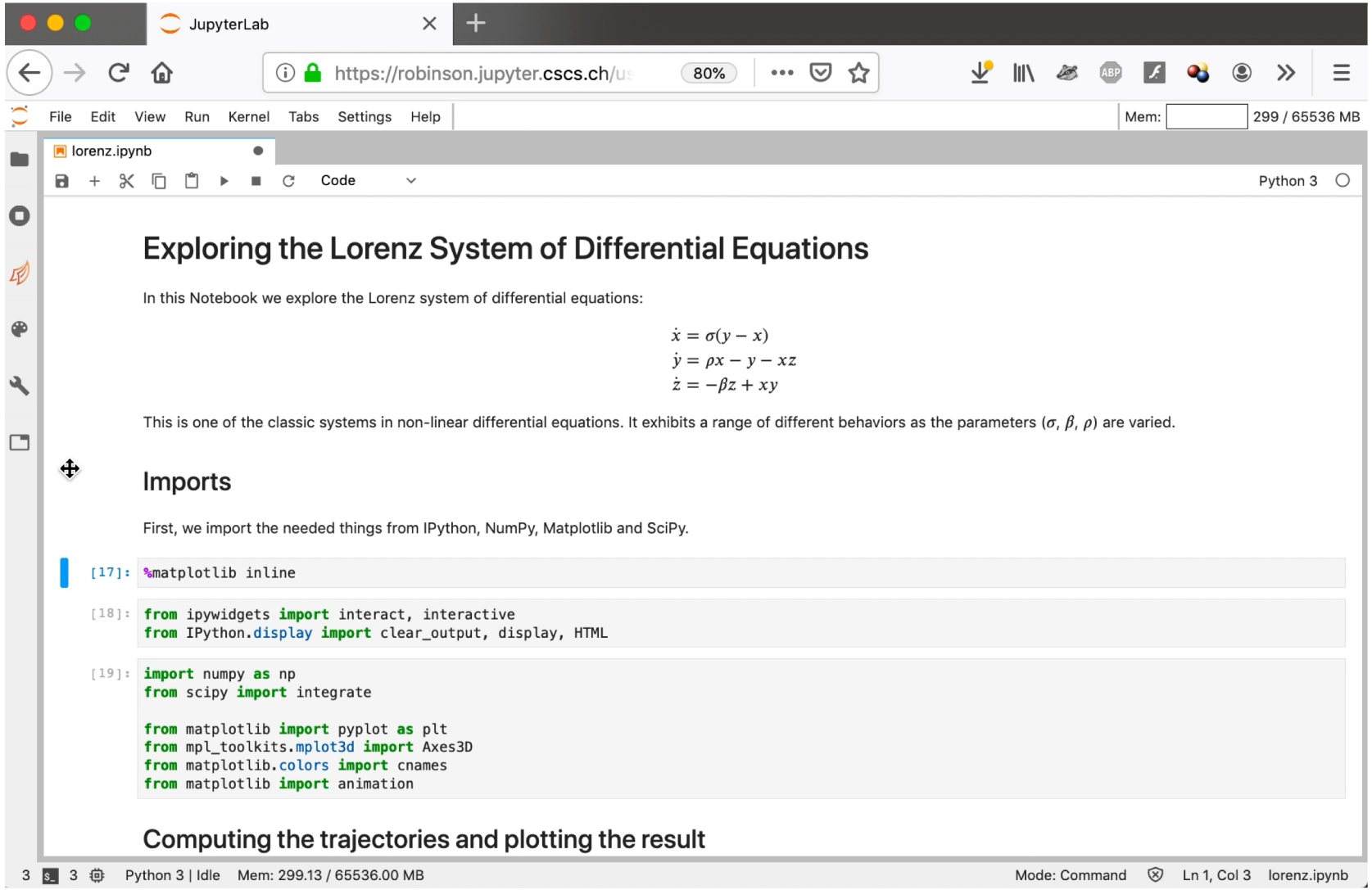
- Next-generation web-based user interface for Jupyter
- Provides higher degree of interaction between notebooks, documents, text editors and other activities (arrange with tabs/splitters)
- Advanced interactive development environment
- Served from same server and uses same notebook document format
- JupyterLab available to the User Lab since March, 2019 (version 0.35.2)
- Upgraded to version 1.1.1 in September 2019

Evolution of Jupyter Notebook to JupyterLab

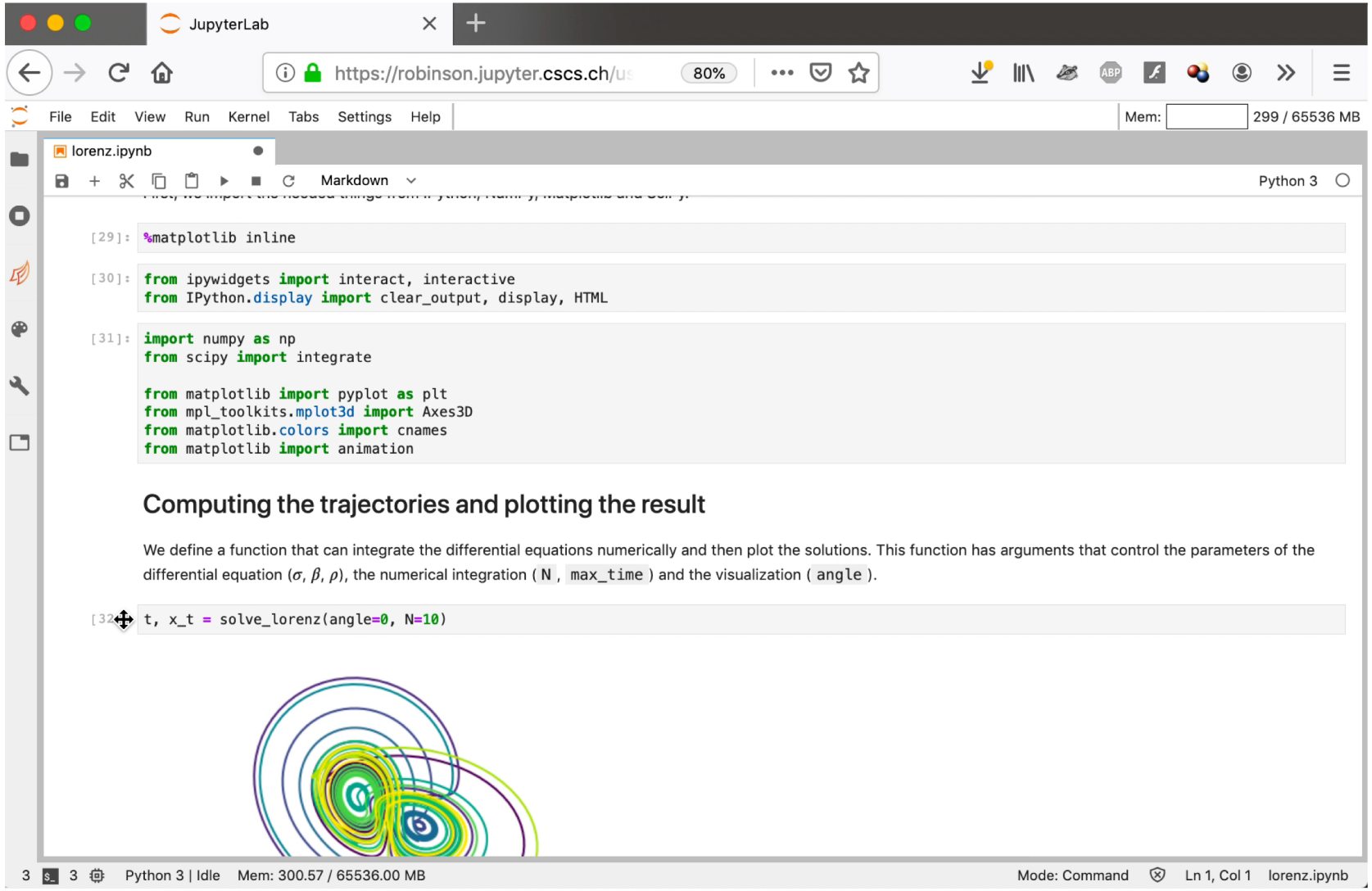




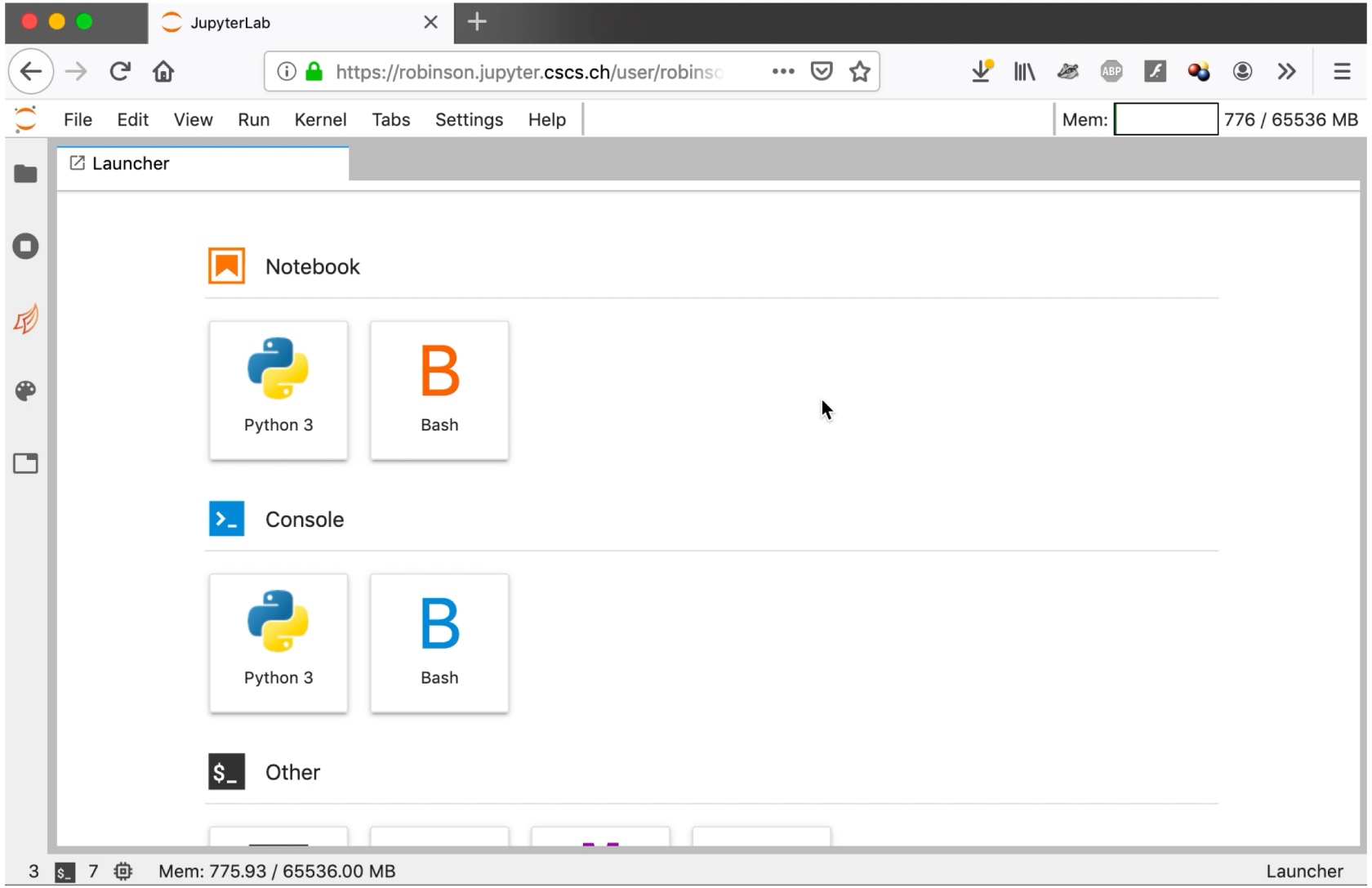
Expand and collapse cells



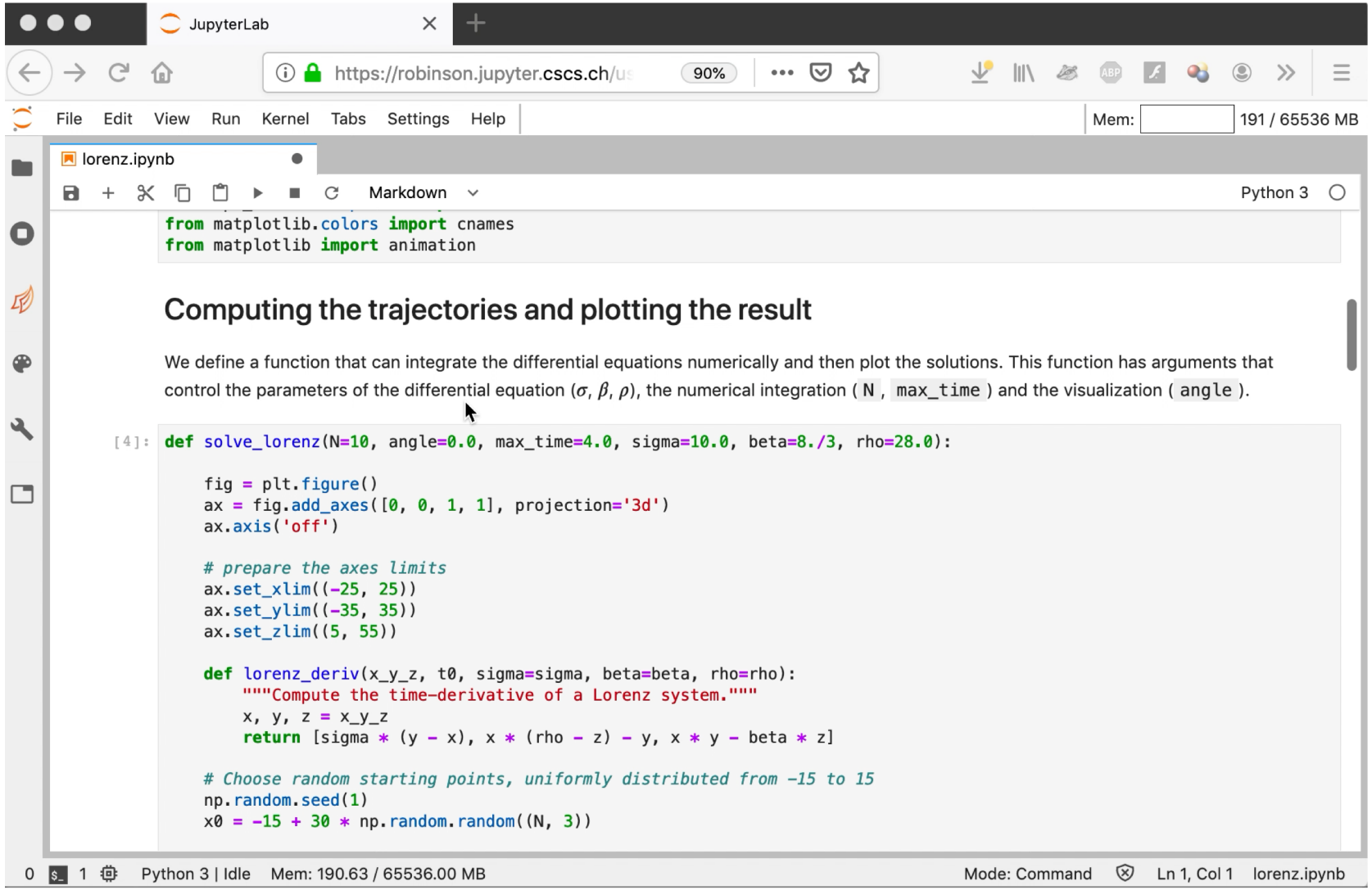
Drag and drop cells with a notebook



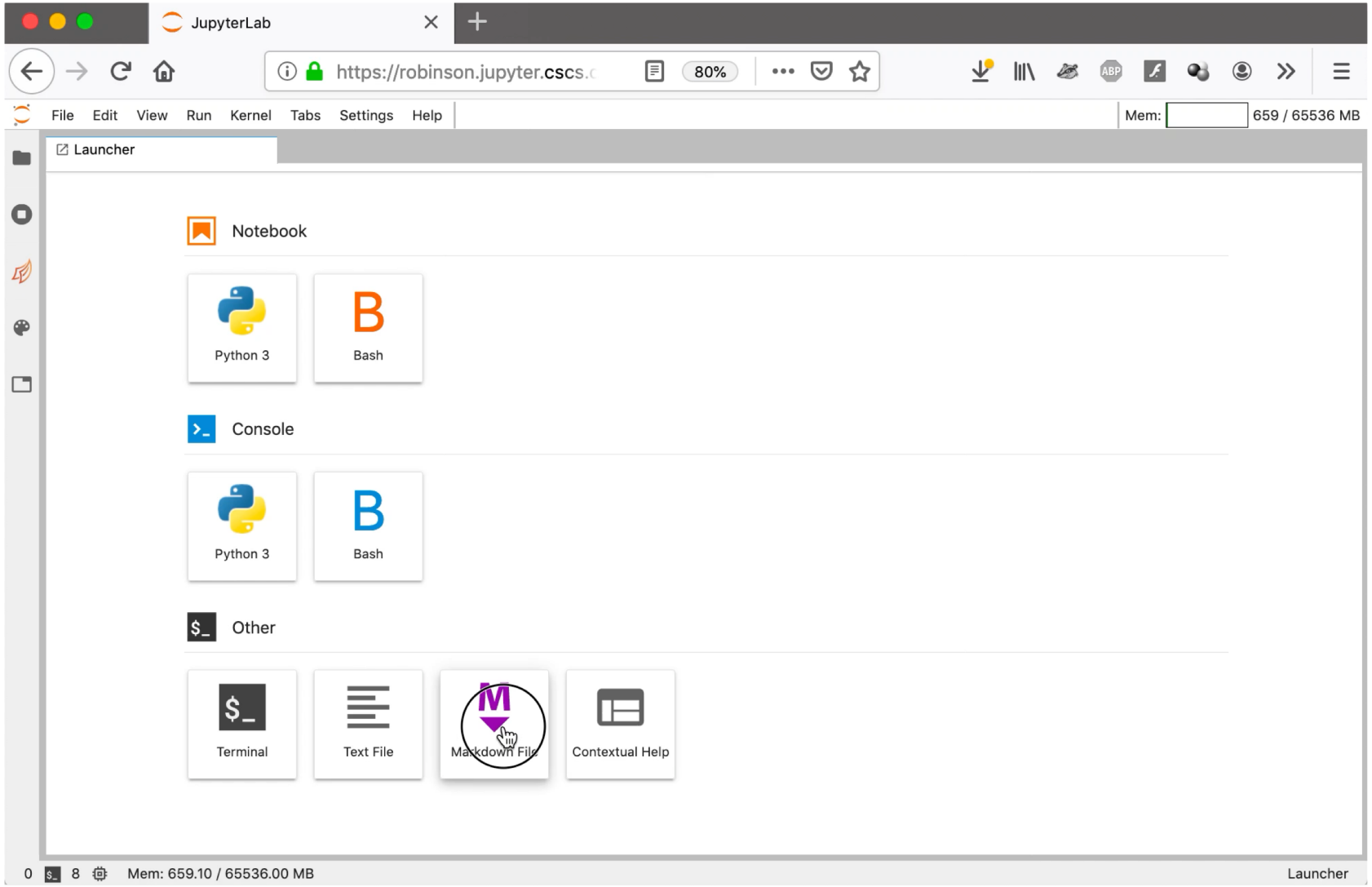
Tab autocompletion in the text editor



Interactive computing – new output view



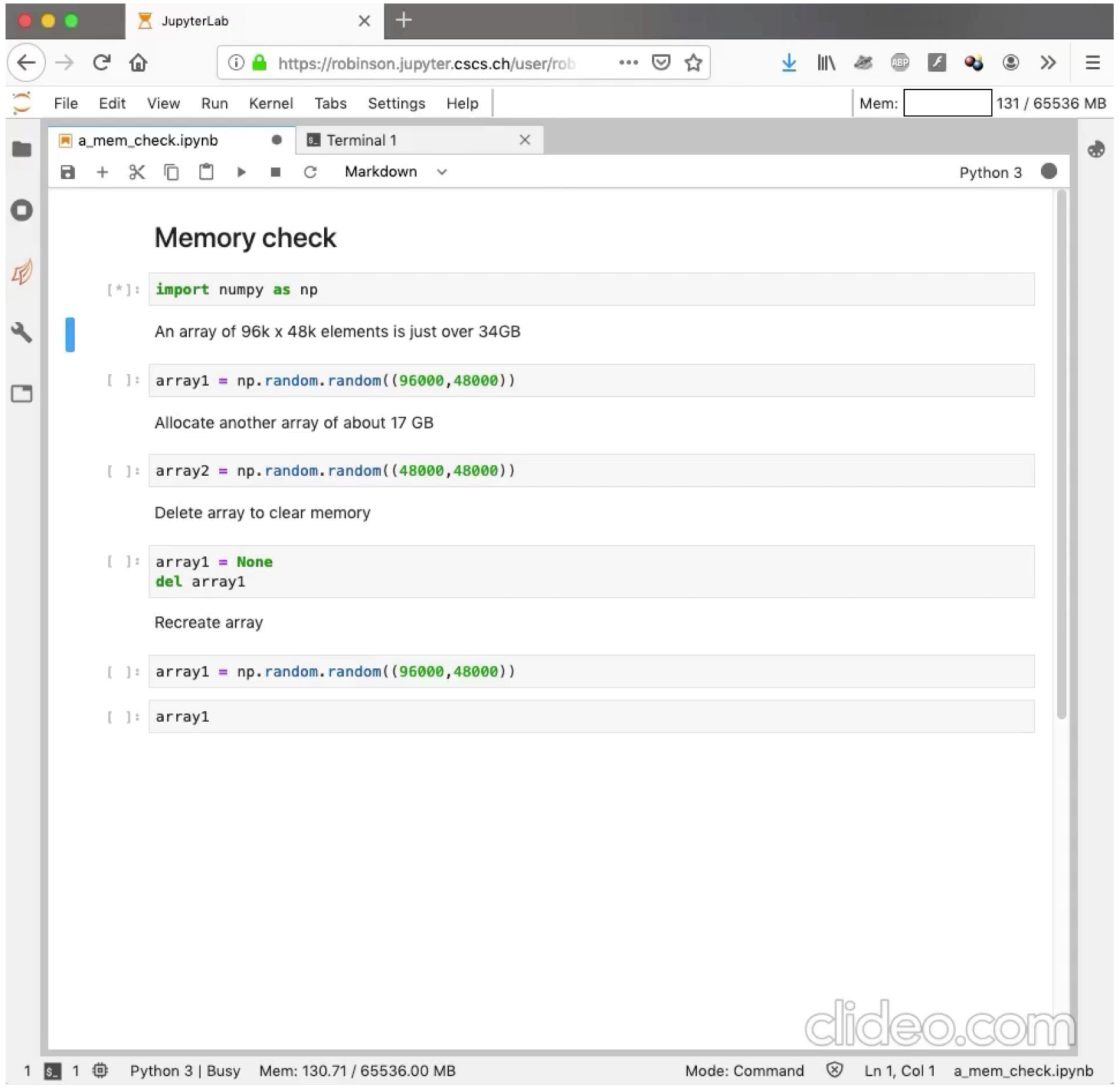
Simplifying code documentation



New extensions enabled with JupyterLab 1.1.1

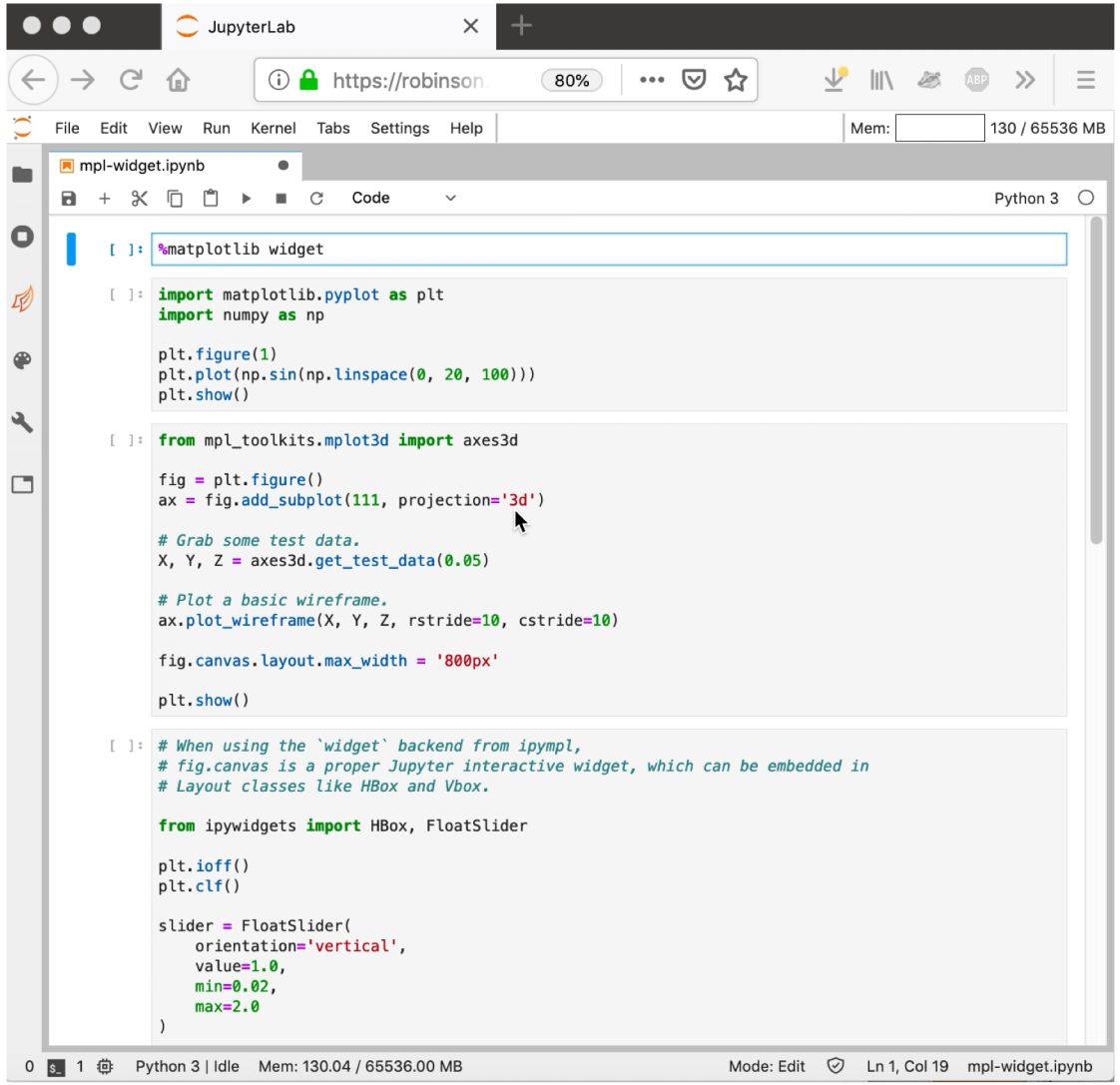
JupyterLab system monitor

- JupyterLab extension to display system information
- Provides a frontend for the *nbresuse* package
- Currently limited to memory usage
- CPU usage and other metrics may be added in the future



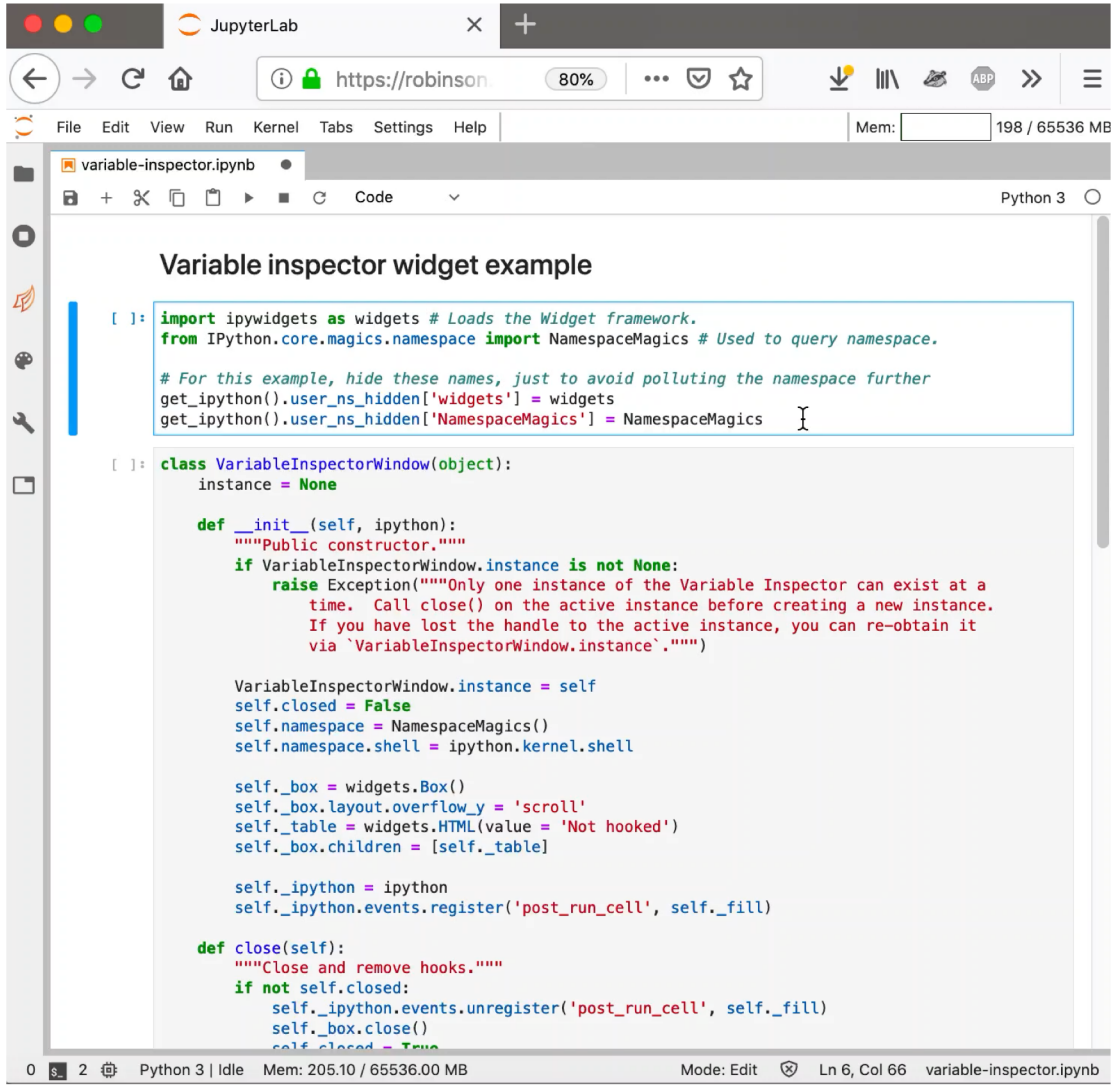
jupyter-matplotlib widgets

- Matplotlib is a commonly used 2D plotting library for producing figures in hardcopy formats, and interactive environments across platforms
- Jupyter-matplotlib enables the interactive features of matplotlib in JupyterLab
- The figure canvas element is a Jupyter interactive widget that can be positioned in interactive widget layouts
- `%matplotlib widget`



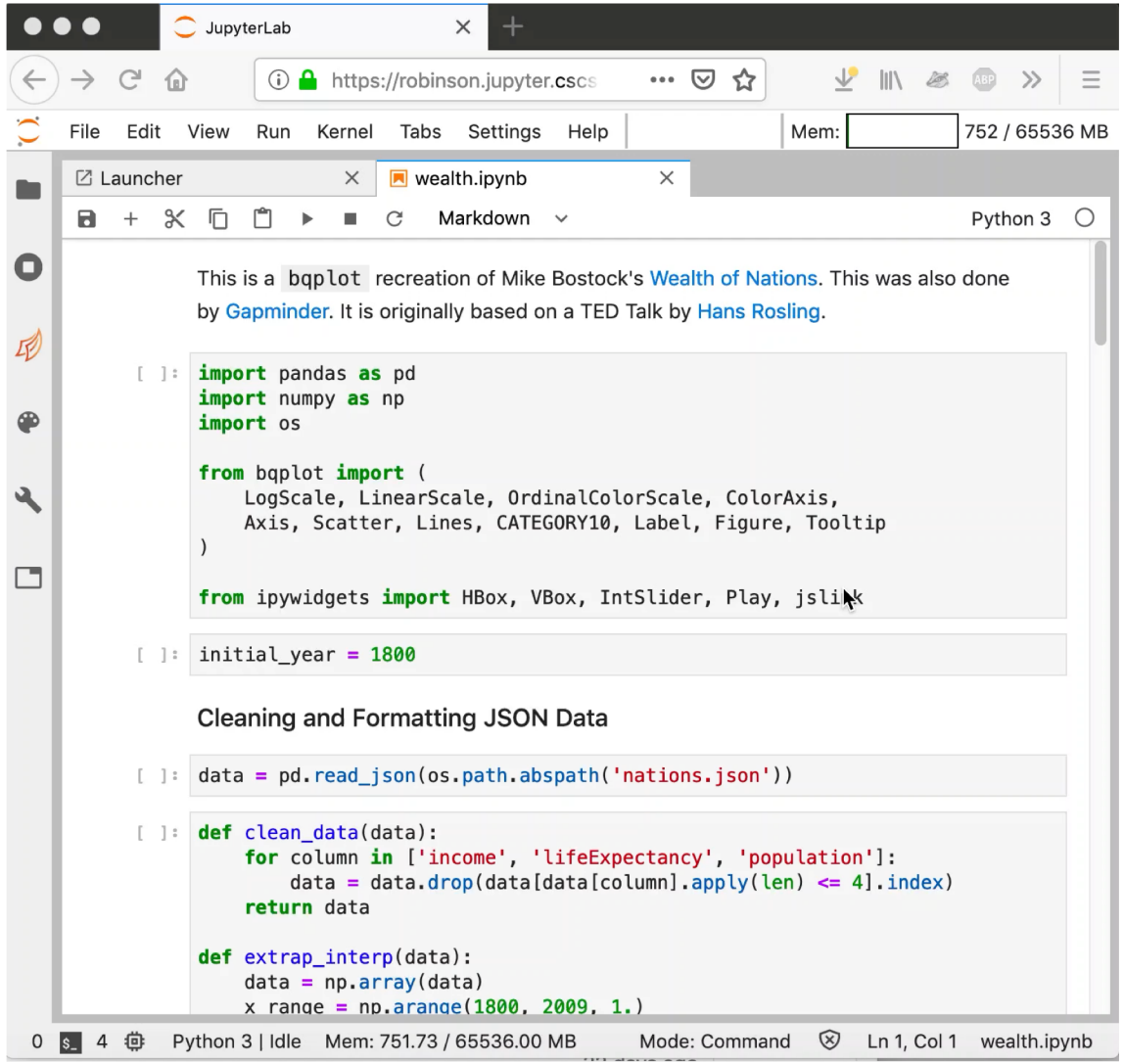
ipywidgets

- Ipywidgets are interactive HTML widgets for Jupyter notebooks and the IPython kernel
- Core widgets
  - Sliders
  - Progress bars
  - Text boxes
  - Toggle buttons and checkboxes
  - Display areas
- Besides the widgets already provided with the library, the framework can be extended with custom widget libraries



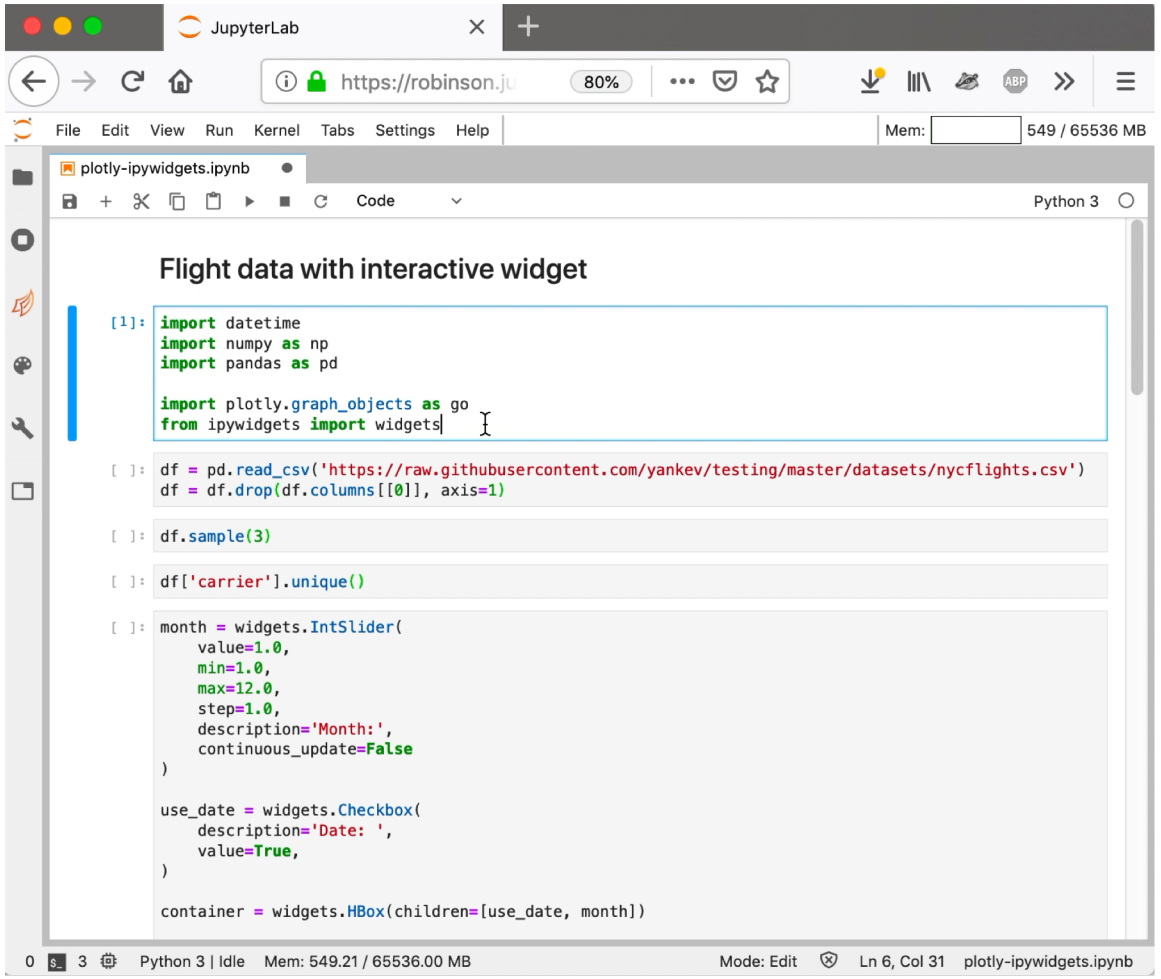
bqplot

- 2D interactive plotting framework for the Jupyter notebook
- In bqplot, every component of a plot is an interactive ipython widget – this means after a plot is drawn you can change almost any aspect of it
- Offers a bridge between Python and d3.js, allowing the ability to build complex interactive GUIs
- Two APIs:
  - Simple “matplotlib inspired” pyplot
  - More verbose API which exposes every element of a plot individually



plotly widgets / jupyterlab-plotly

- plotly.py is an interactive graphing library for Python
- Over 30 chart types (scientific charts, 3D graphs, statistical charts, SVG maps, financial charts,…)
- Plotly 3.0.0 introduced a new Jupyter widget class for notebook and JupyterLab: `plotly.graph_objs.FigureWidget`

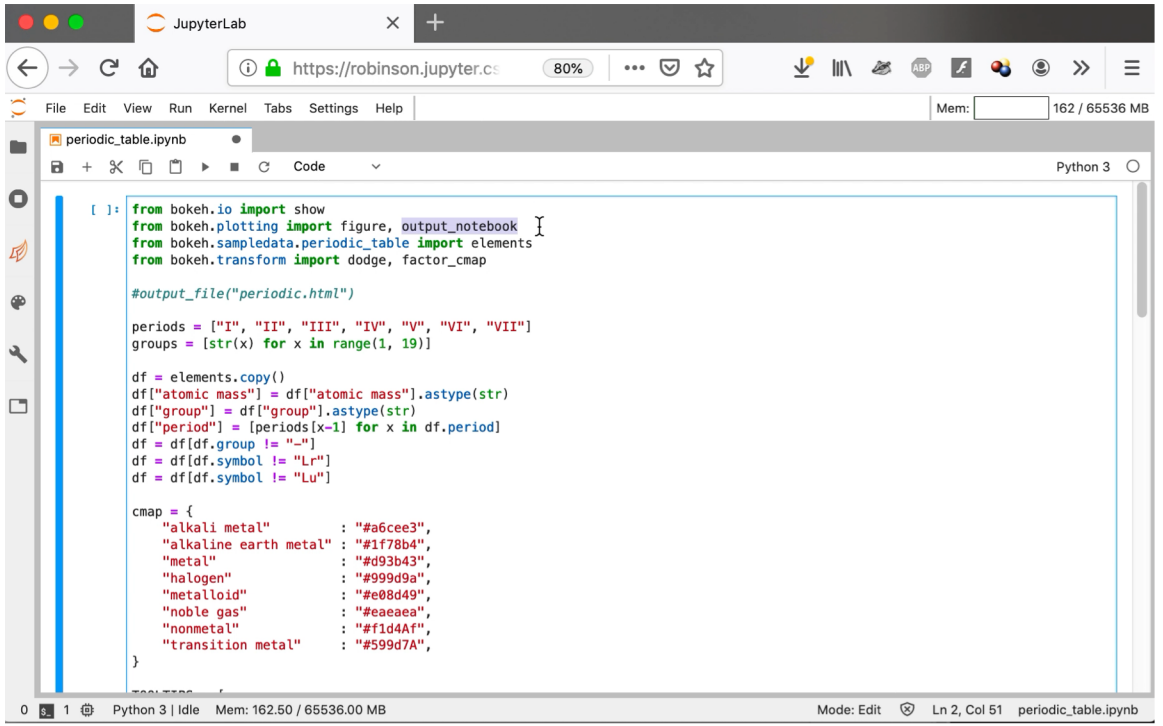


Jupyterlab_bokeh

- Bokeh is an interactive visualization library for Python that enables visual presentation of data in web browser
- With Bokeh, you can create interactive plots, dashboards, and data applications

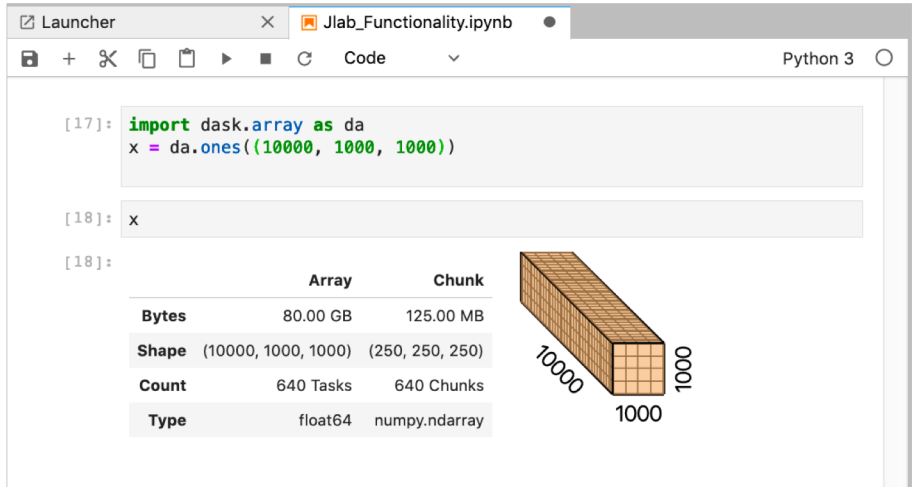
jupyterlab_bokeh

- Bokeh is an interactive visualization library for Python that enables visual presentation of data in web browser
- With Bokeh, you can create interactive plots, dashboards, and data applications
- Jupyterlab_bokeh is a server extension for rendering this content in JupyterLab

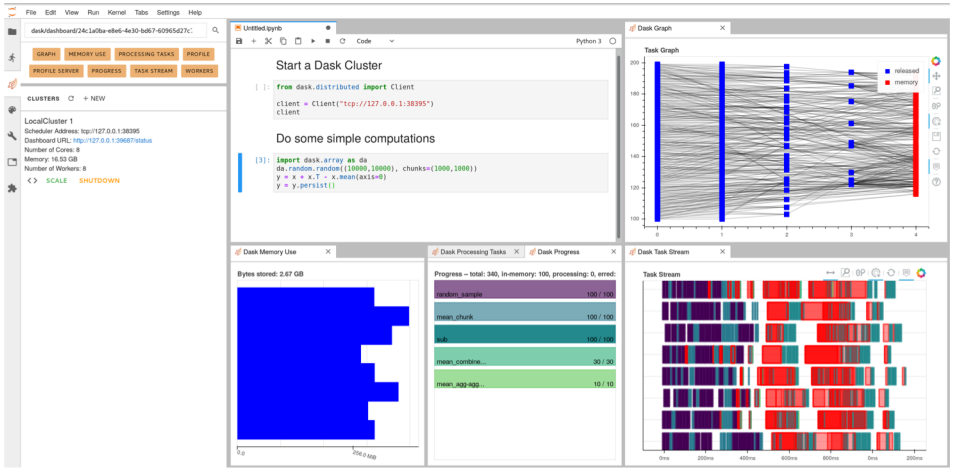


Dask and dask JupyterLab extension

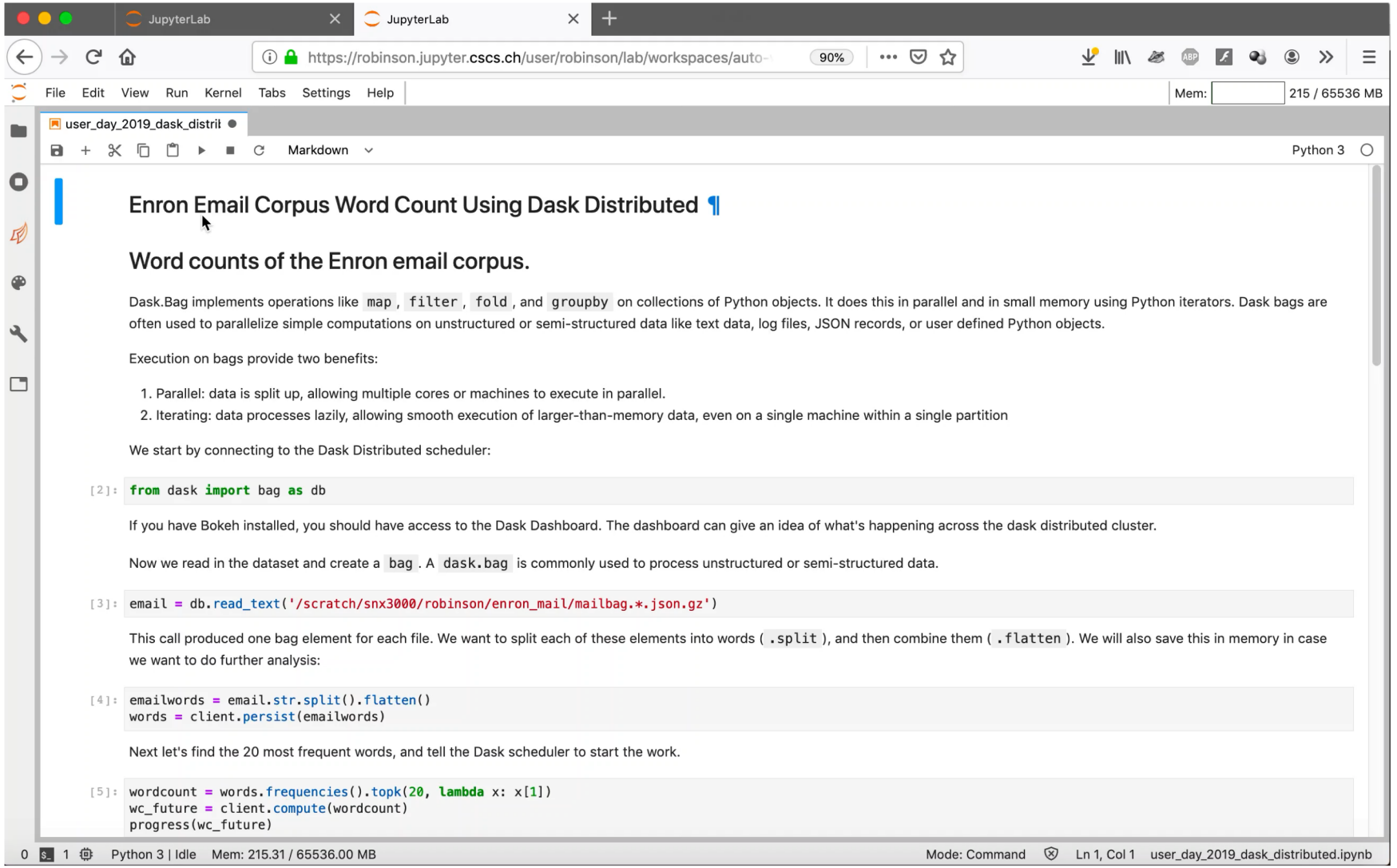
- Dask is a flexible library for parallel computing in Python
- Extends interfaces like *NumPy, Pandas, or Python iterators* to larger-than-memory / distributed environments
- These parallel collections run on top of dynamic task schedulers



- Dask JupyterLab extension to manage Dask clusters, as well as embed Dask's dashboard plots directly into JupyterLab panes



Dask JupyterLab extension



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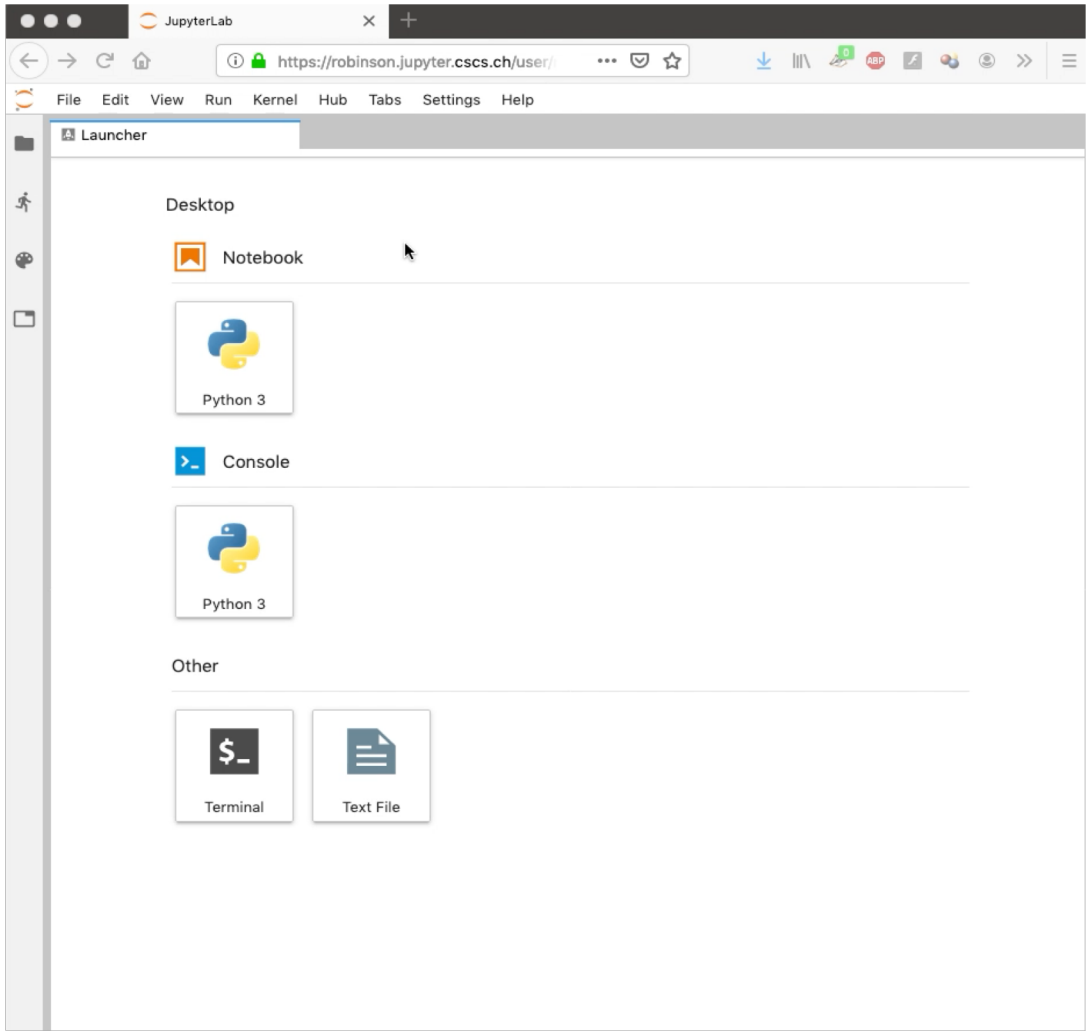
Changes and New Functionality in JupyterLab 1.0+

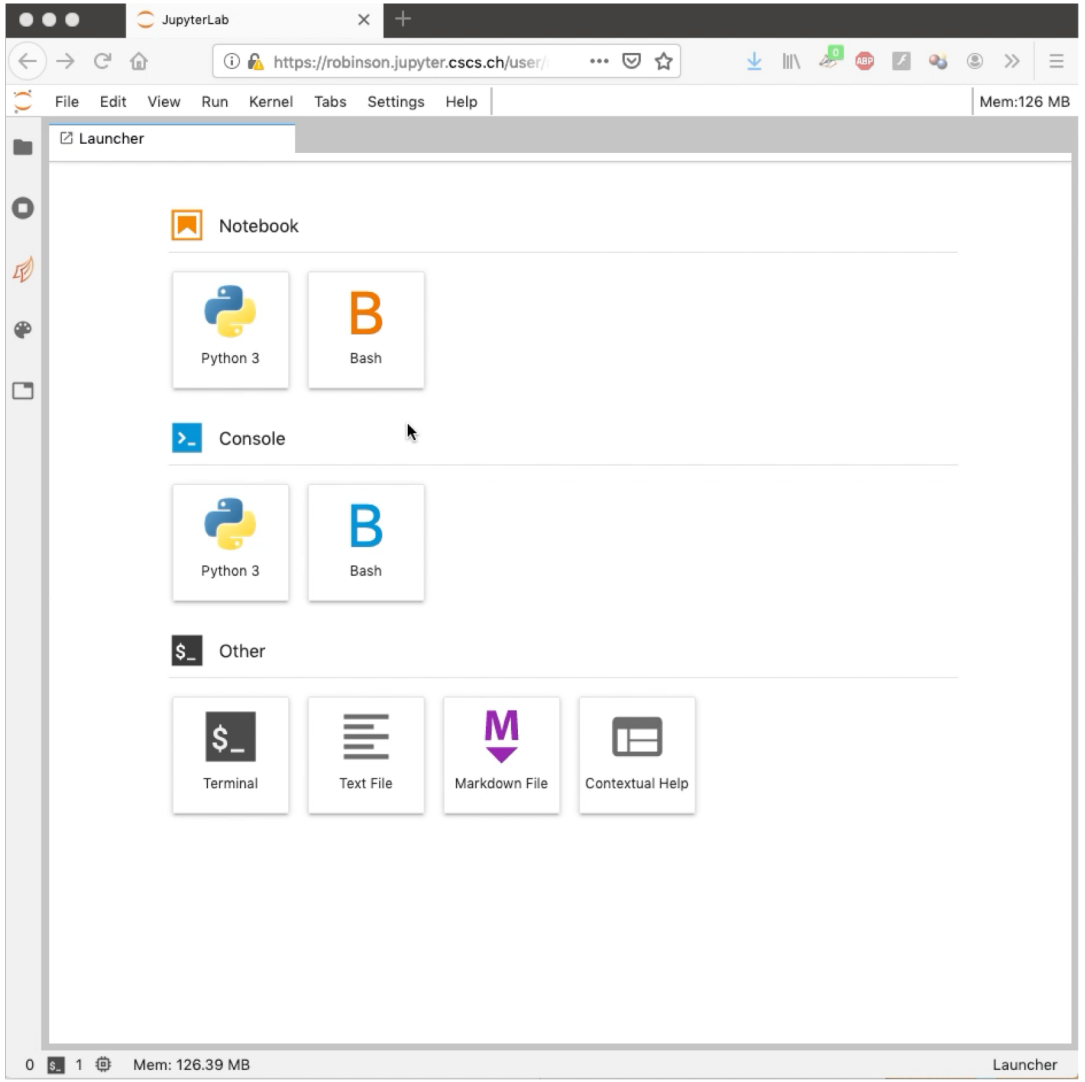
JupyterHub integration

- Previously, to stop your server you needed to use Hub > Control Panel



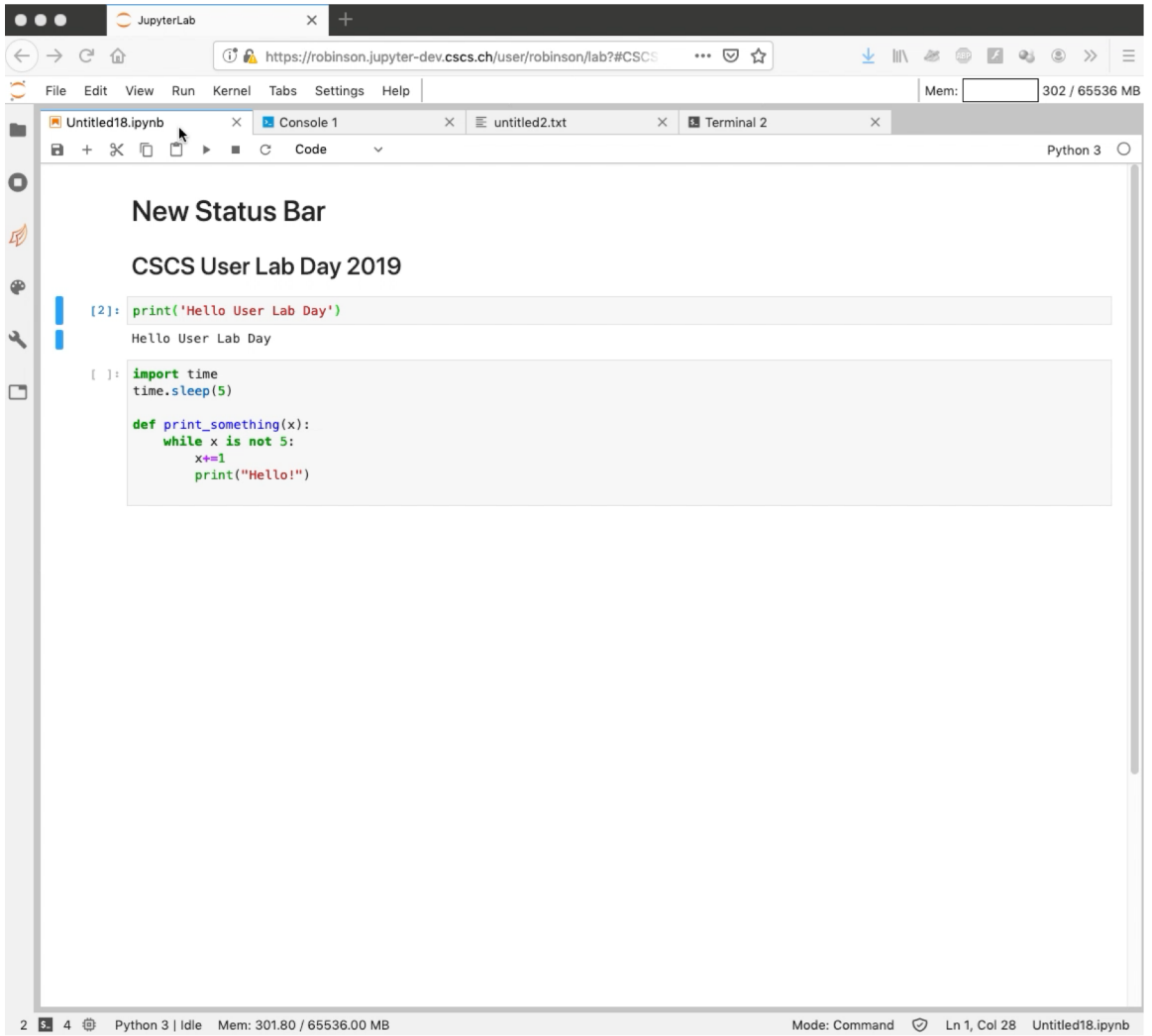
JupyterHub integration

- Previously, to stop your server you needed to use Hub > Control Panel
- Now, the JupyterHub extension is included in the core JupyterLab distribution
- To stop your sever: File > Control Panel
- Note: File > Logout will not stop your server!



Status bar

- Jupyterlab-statusbar provides a generic status bar to showcase the various states of JupyterLab
- Different components render depending on the active context: notebook, console, file editor, and terminal
- Can be used by other extensions to add custom elements into the status bar



Status bar (2)

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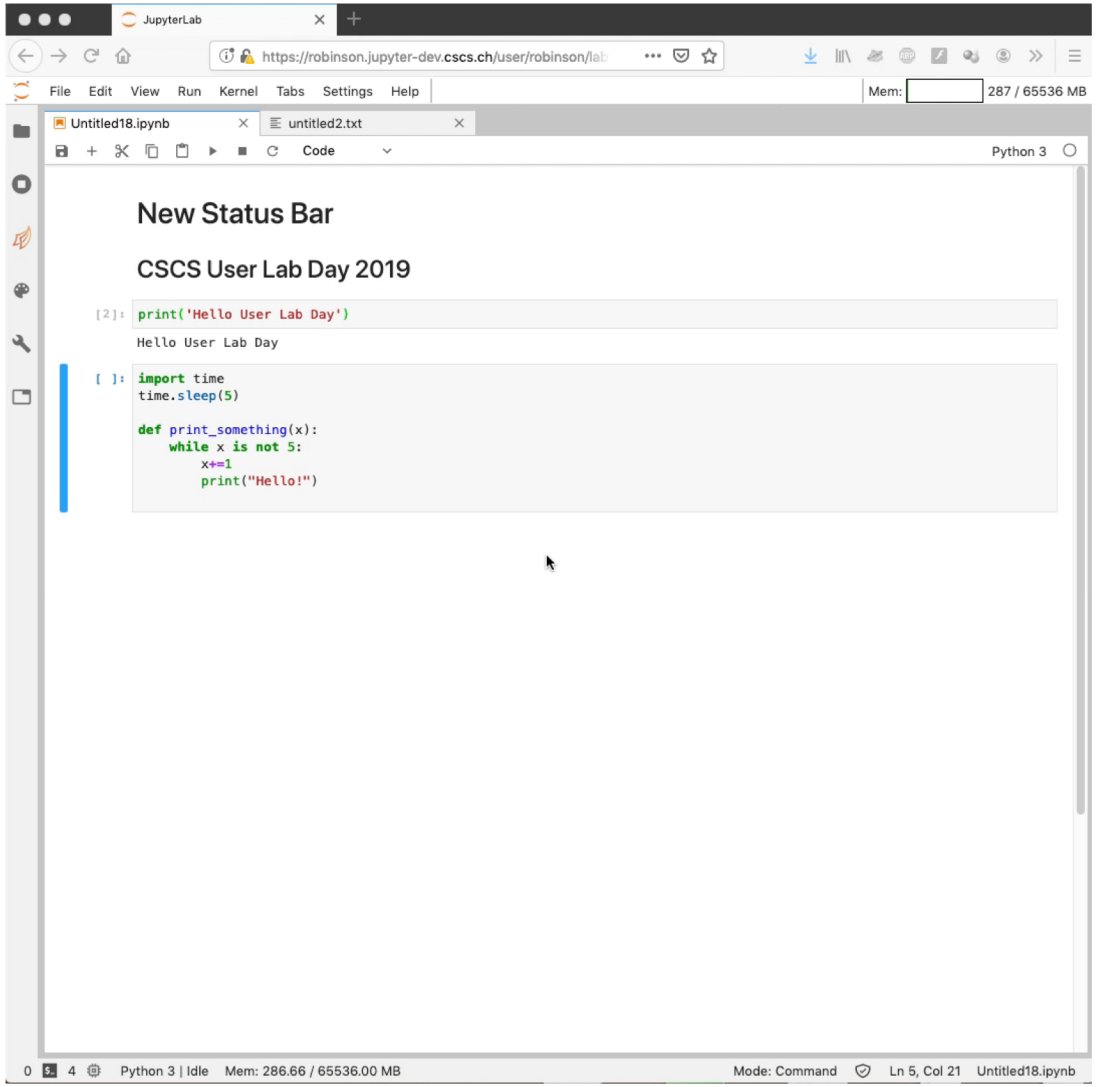
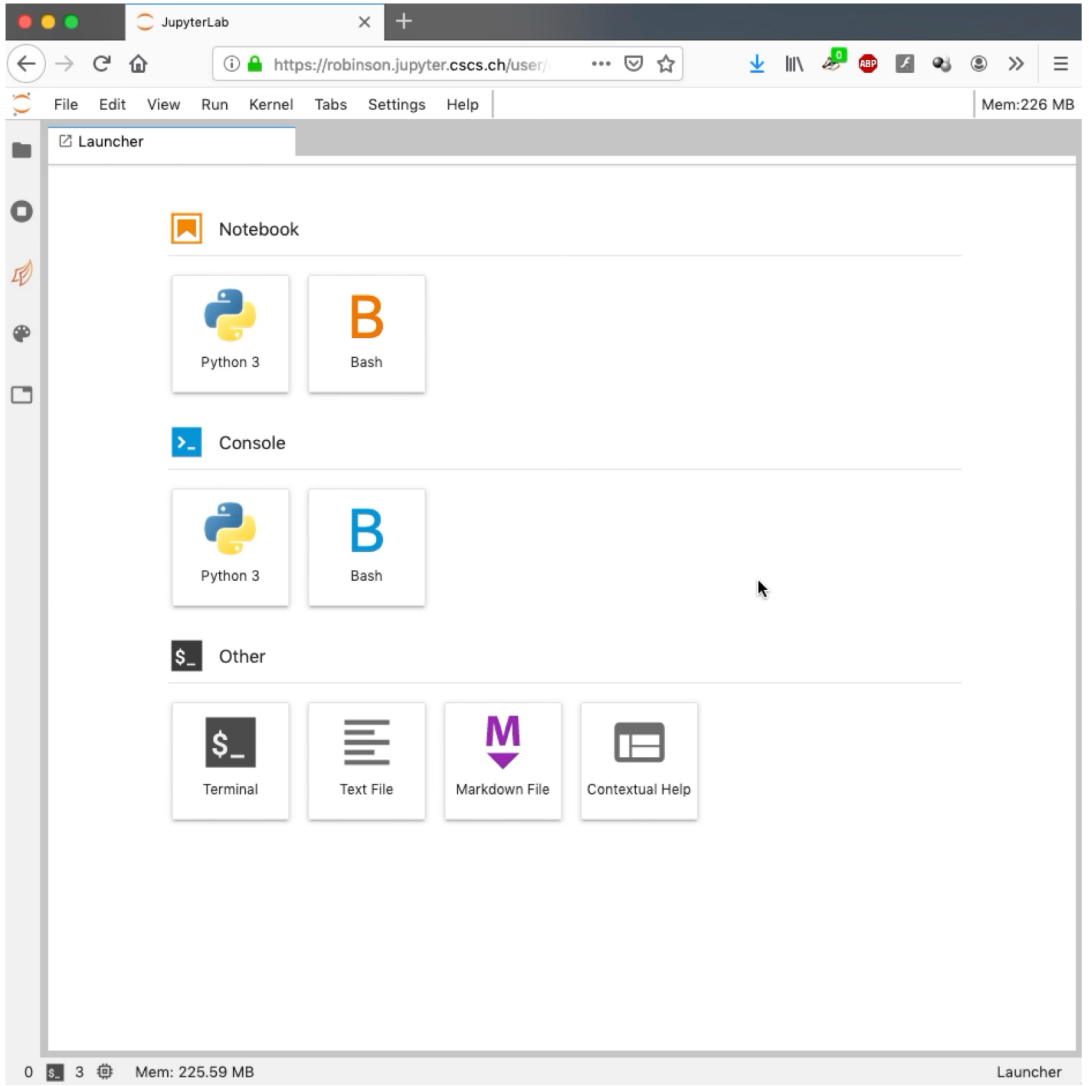


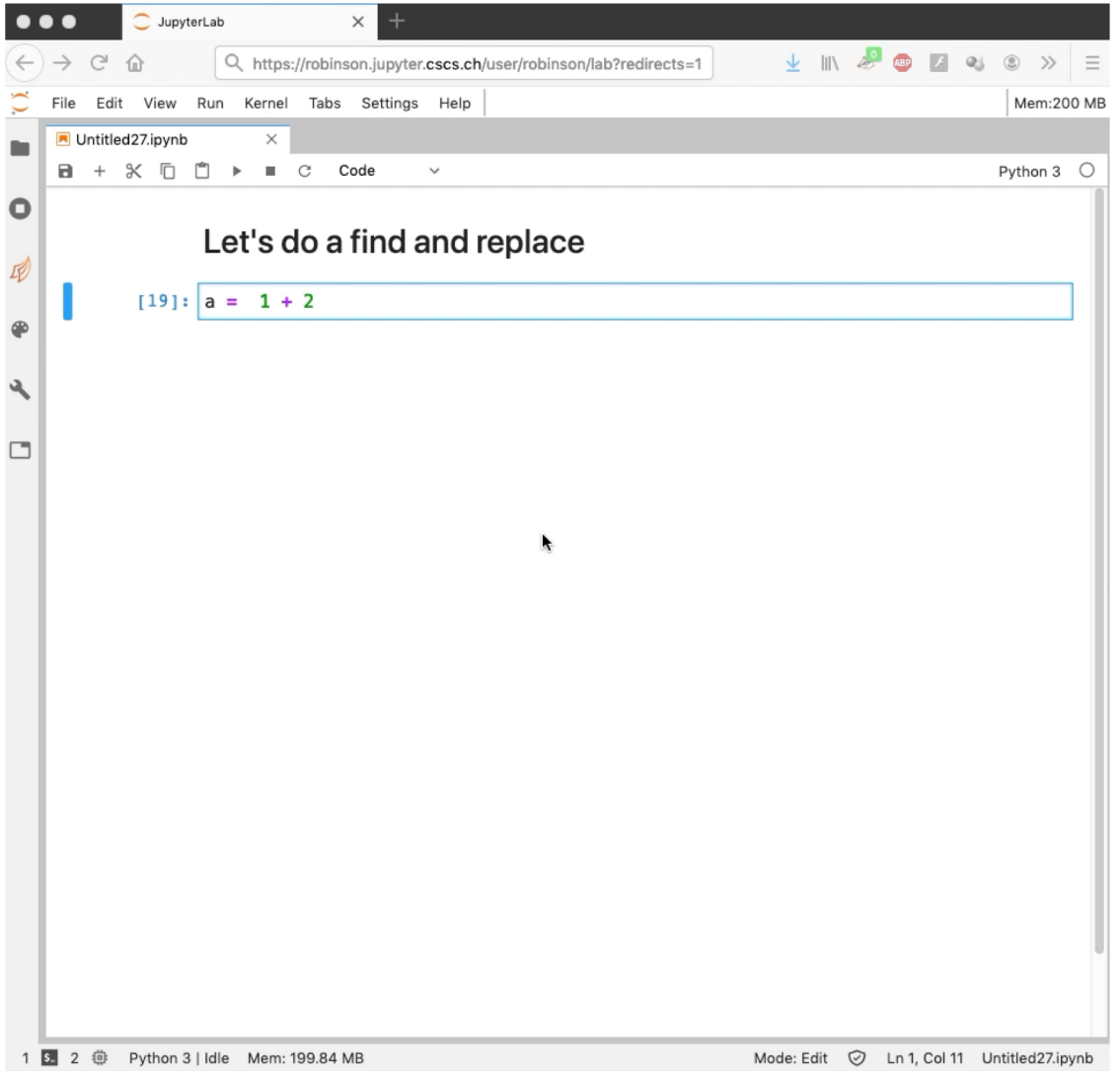
New kernels

- Bash kernel now available in the launcher
- IJulia kernel *coming soon…*



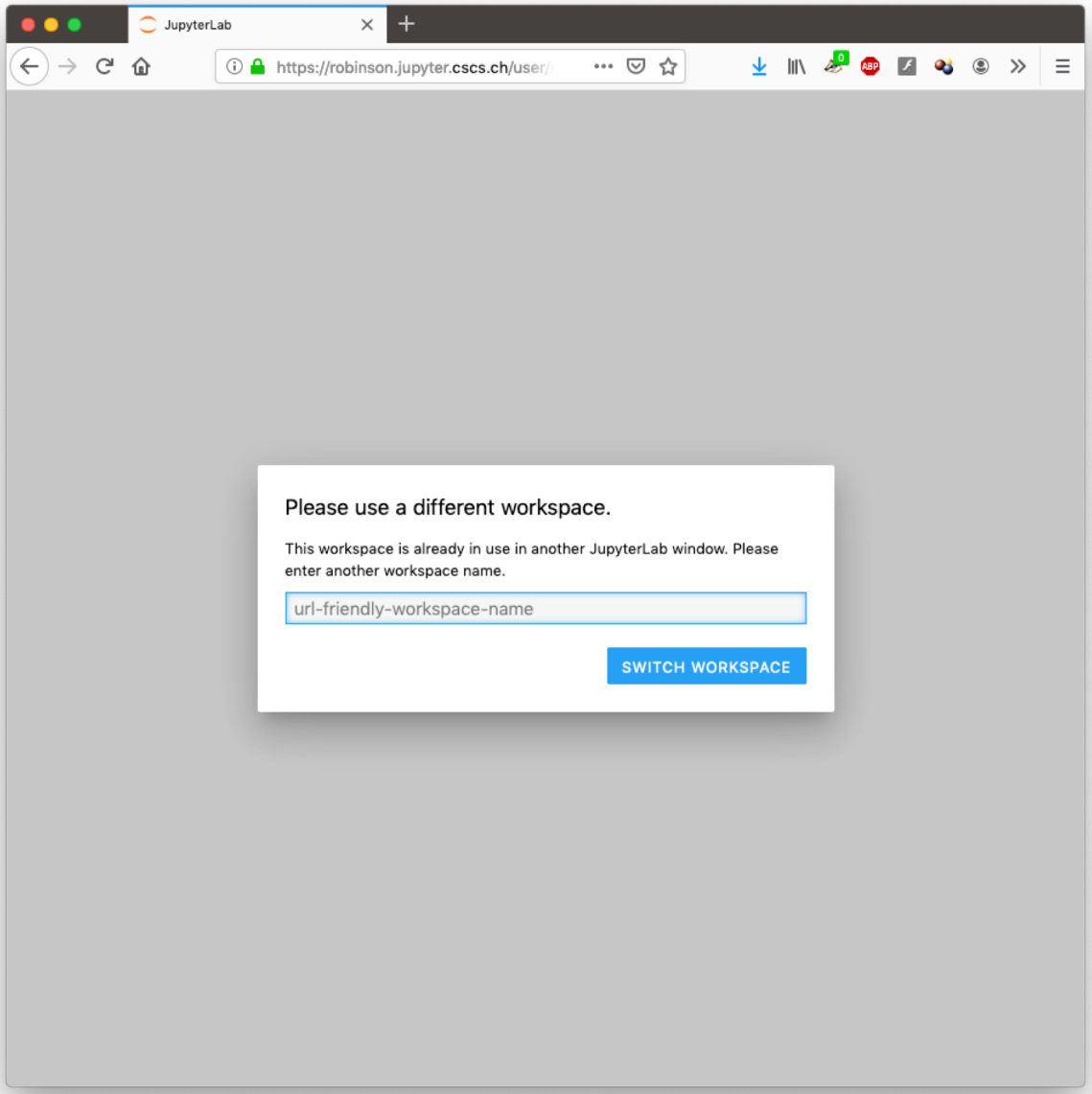
Find and replace

- First class support for find and replace across JupyterLab
- Currently works in notebooks and text files
- Supports regex
- Extensible to other widgets



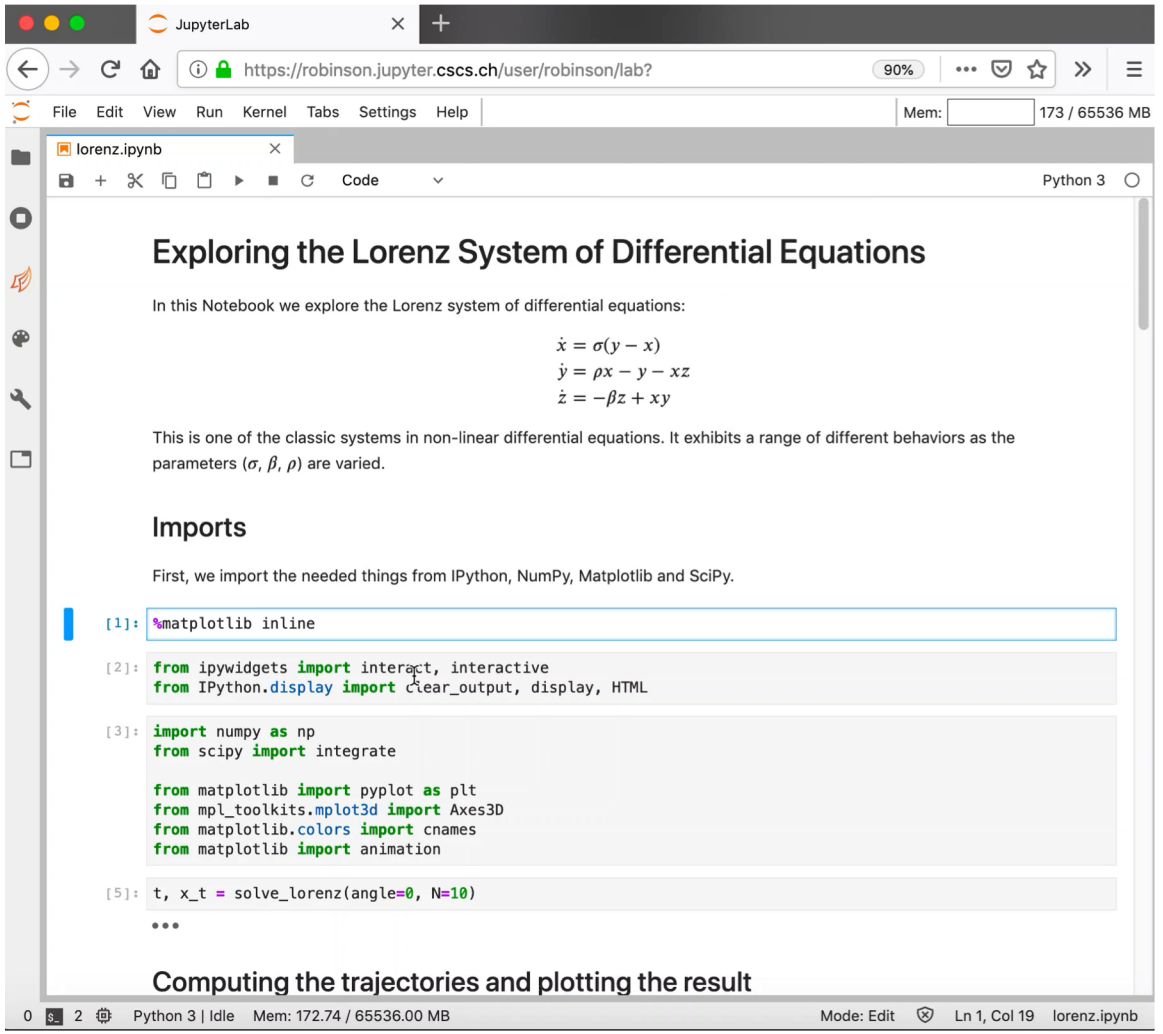
New workspaces are auto-generated

- Previously, you would receive an annoying pop-up message ***Please use a different workspace*** if you have a workspace open in another browser tab



New workspaces are auto-generated

- Previously, you would receive an annoying pop-up message ***Please use a different workspace*** if you have a workspace open in another browser tab
- Now, **new workspaces are automatically generated** when you create a new window with the same workspace name
- User is redirected to a randomly generated workspace name of the form auto-*x* where *x* is randomly drawn from [A-Z,a-z,0-9].



Other User Facing Changes in JupyterLab 1.X

- “Inspector” is renamed “Contextual Help” and is moved to the Help menu
- Drag and drop notebook cells into console or text editor
- Command to render all markdown cells
- Ability to “Merge Selected Cells” in the context menu
- Notification when a kernel is automatically restarted, e.g., out-of-memory crash
- Many other changes to the user interface; various bug fixes

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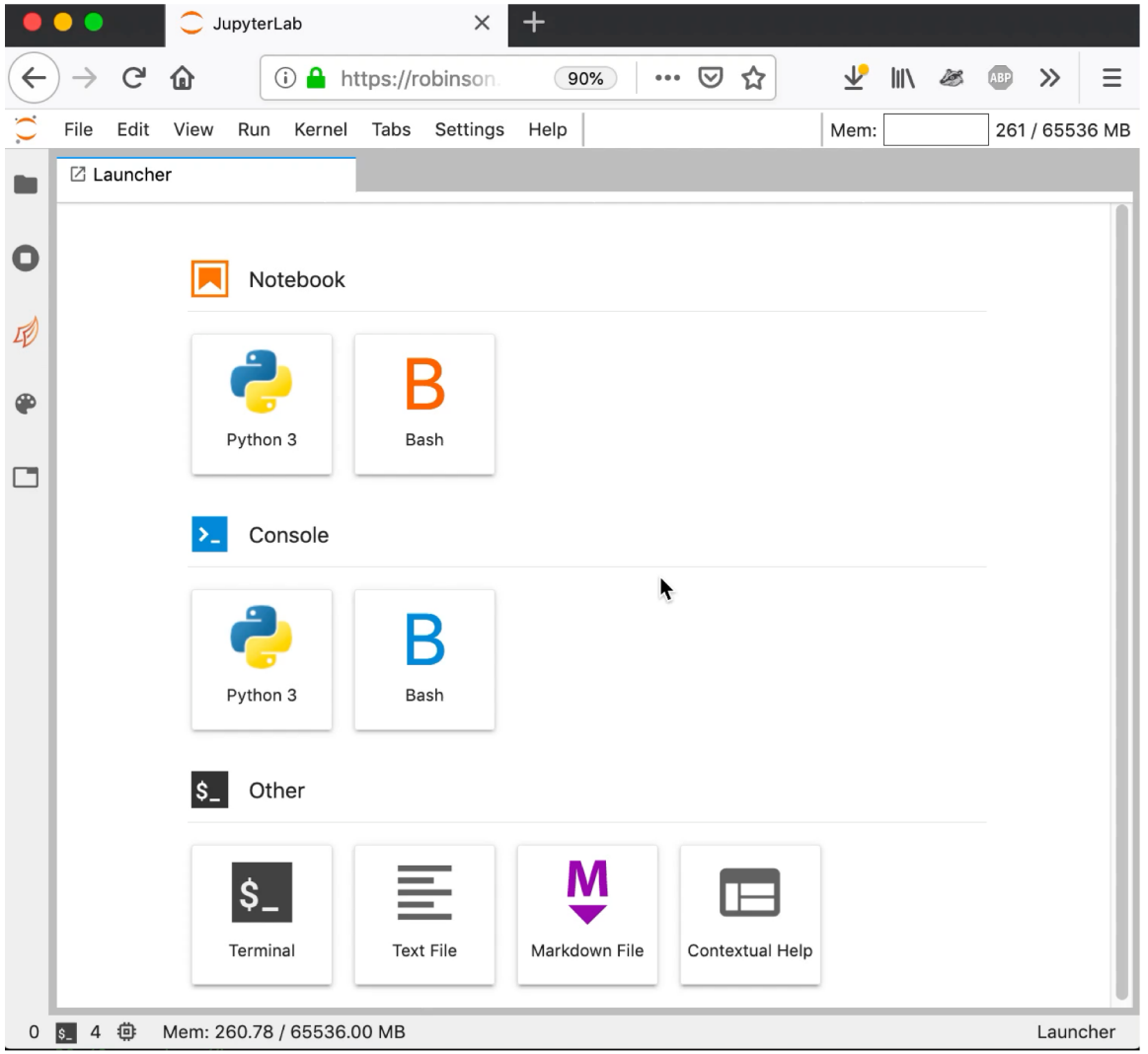
New Functionality in JupyterHub 1.0

Named servers

- In addition to your default server, you can now have additional server(s) with names
- This allows you to have more than one server running at the same time
- For example, you might want one server running on a “gpu” node, and another server on an “mc” node
- Managed through a new user interface



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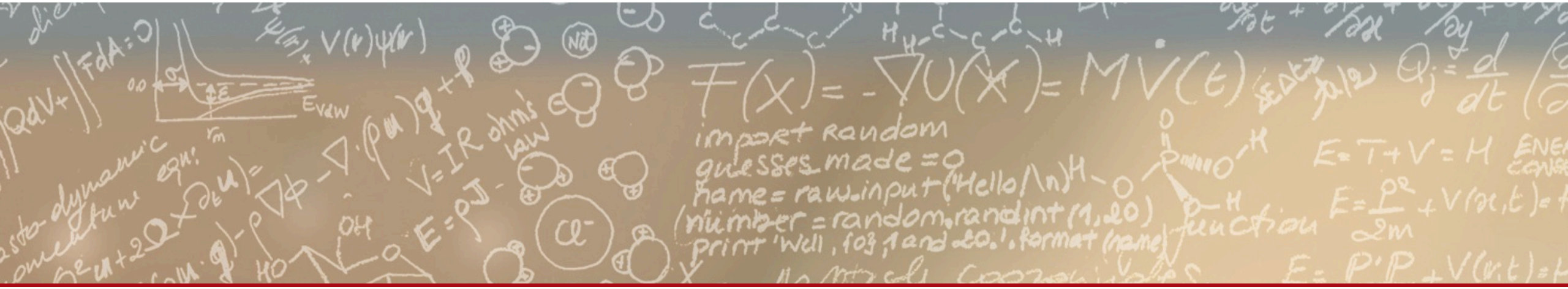

Thank you. We welcome your feedback on the Jupyter service!

help@cscs.ch

Coming soon: survey on interactive computing use & requirements