



## Benefits and Limitations of Jupyter-based Web Applications

Nicole Brewer, Rajesh Kalyanam, Rob Campbell,  
Carol Song, Lan Zhao





## ~~Benefits and Limitations of Jupyter-based Web Applications~~

### “The Story of the Little Notebook”

Nicole Brewer, Rajesh Kalyanam, Rob Campbell,  
Carol Song, Lan Zhao





## Nicole Brewer

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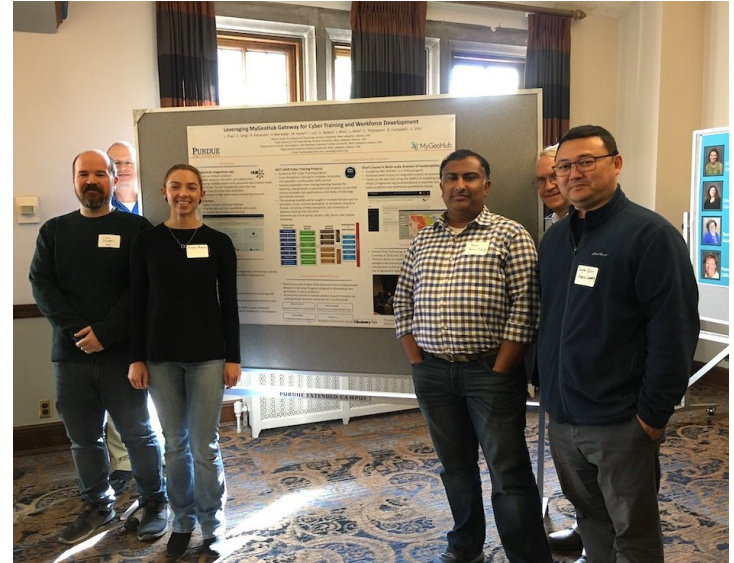


@catch\_me\_coding



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# Overview

1. What is a scientific web application?
2. Why should researchers develop them?
3. How should researchers and RSEs collaborate?
4. When should RSEs build apps with Jupyter Notebooks?
  - a. Benefits
  - b. Deployments and supported features
  - c. Limitations
  - d.

# What is a scientific web application?

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A scientific application is a graphic interface that **allows users to manage and analyze data and perform computations**

Landing Estimates Results Settings

Model Class Analysis of Variance

Factors 1

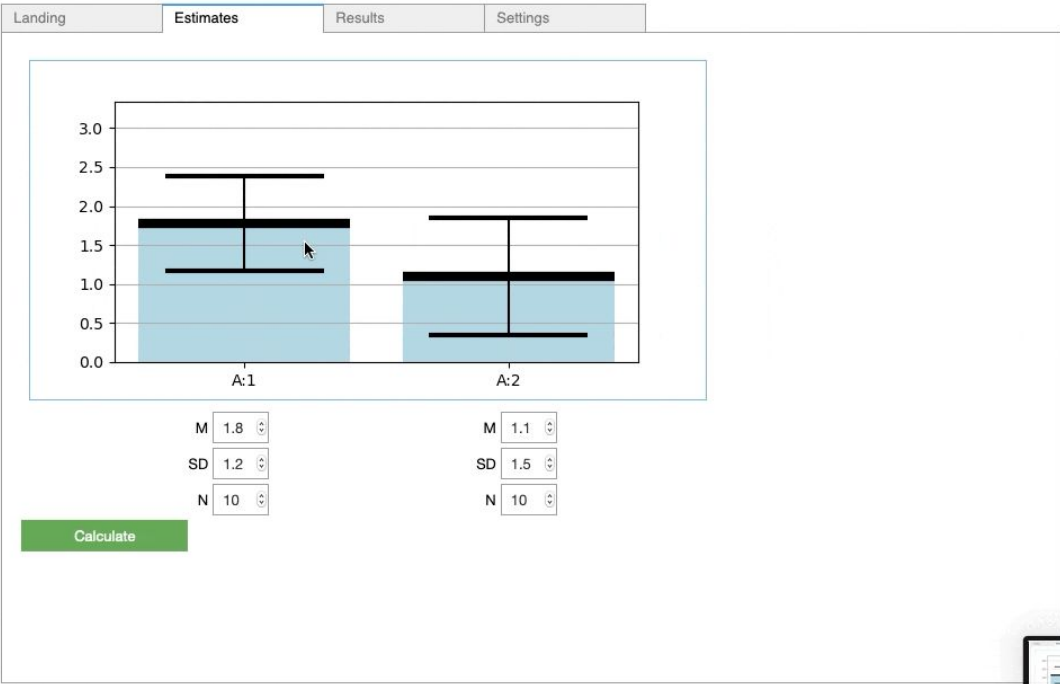
Factor A Levels 2 1 2

☒ Between  
☐ Within

Covariates 0

Proceed

A scientific application is a graphic interface that **allows users to manage and analyze data and perform computations**





A scientific application is a graphic interface that **allows users to manage and analyze data and perform computations**

Landing

Estimates

Results

Settings

ID	Name	Date	Runtime	Input
1618000161492	powerANOVAS	2021-04-09 16:29:21	8.47338795	{'N': [[10, 10]], 'SDs': [array([1.8, 1.5
1618000162551	powerANOVAS	2021-04-09 16:29:22	0.99832201	{'N': [[10, 10]], 'SDs': [array([1.8, 1.5

```
{'pairwise_p': 0
0 0.0,
'design_attributes': {'N': array([10, 10], dtype=int32),
'means': {'A': array([1.05244067, 1.1      ])},
'SDs': array([1.8, 1.5]),
'corr': None,
'covMat': None,
'labels_factors': 'A',
'labels_levels': {'A': ['1', '2']},
'num_factors': 1,
'num_levels': 2,
'factorTypes': 'b'},
'data': 0      1      2      1      2      3      4      5      6  \
0      1      2      1      2      1      2      1
1      ID1      ID2      ID3      ID4      ID5      ID6      ID7
2      1      2      1      2      1      2      1
3      1.0      0.0      1.0      0.0      1.0      0.0      1.0
```

# Why should researchers develop web apps?

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## **Web applications are increasingly popular scientific publication tools**

- Internal tool to improve research process
- Teaching
- Outreach
- Stakeholder engagement
- Updating policy makers on the evolving state of the COVID-19 pandemic

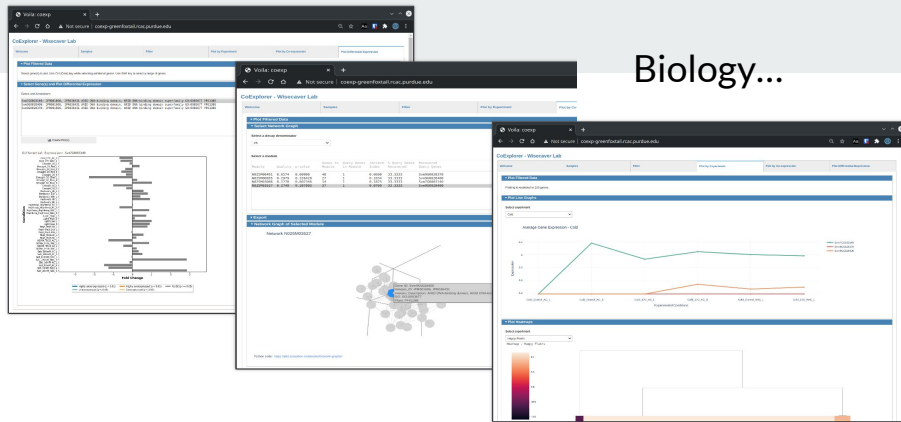


## Web applications improve the quality of research data and software

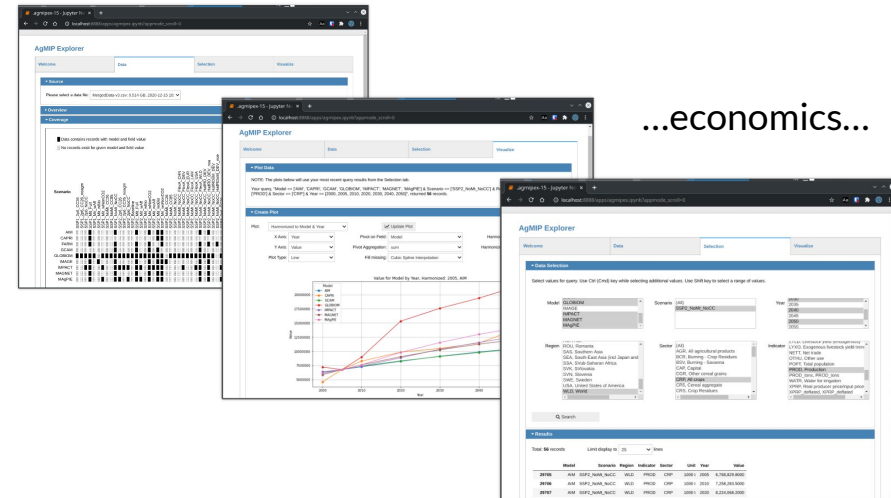
- **Accessibility** of cyberinfrastructure for non-technical users
- **Reusability** of data and software
- **Reproducibility** may be improved depending on the app design

**How should RSEs and  
scientists collaborate?**

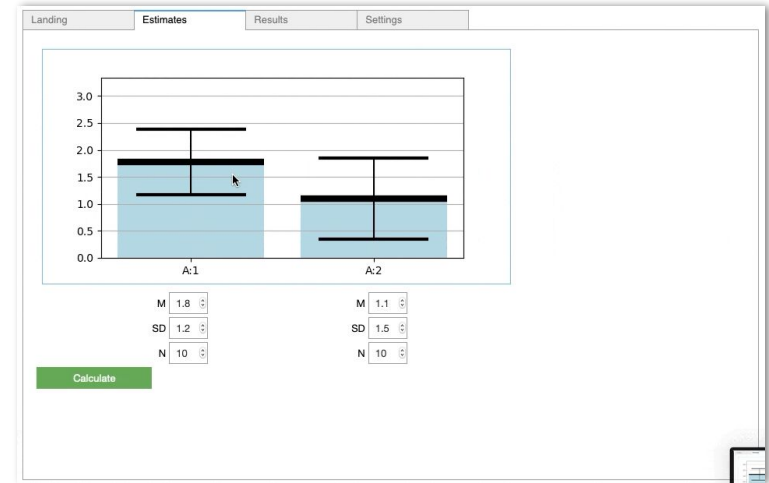
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Biology...



...economics...



...psychology,

aeronautics,

and more.

**When should RSEs use Jupyter  
to develop web apps?**

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# When should RSEs use a Jupyter Notebook?



Benefits	Supported Features	Limitations
<ol style="list-style-type: none"><li>1. scientists may have an existing notebook</li><li>2. easy for researchers to maintain</li><li>3. third-party widget ecosystem</li></ol>	<ul style="list-style-type: none"><li>• Shared Storage</li><li>• User Authentication</li><li>• Group Managment</li><li>• Repeating Components</li></ul>	<ul style="list-style-type: none"><li>• Little stylistic control</li><li>• Third-party widget ecosystem</li><li>• Modularity requires OOP expertise</li><li>• Many data visualization libraries aren't interactive</li></ul>



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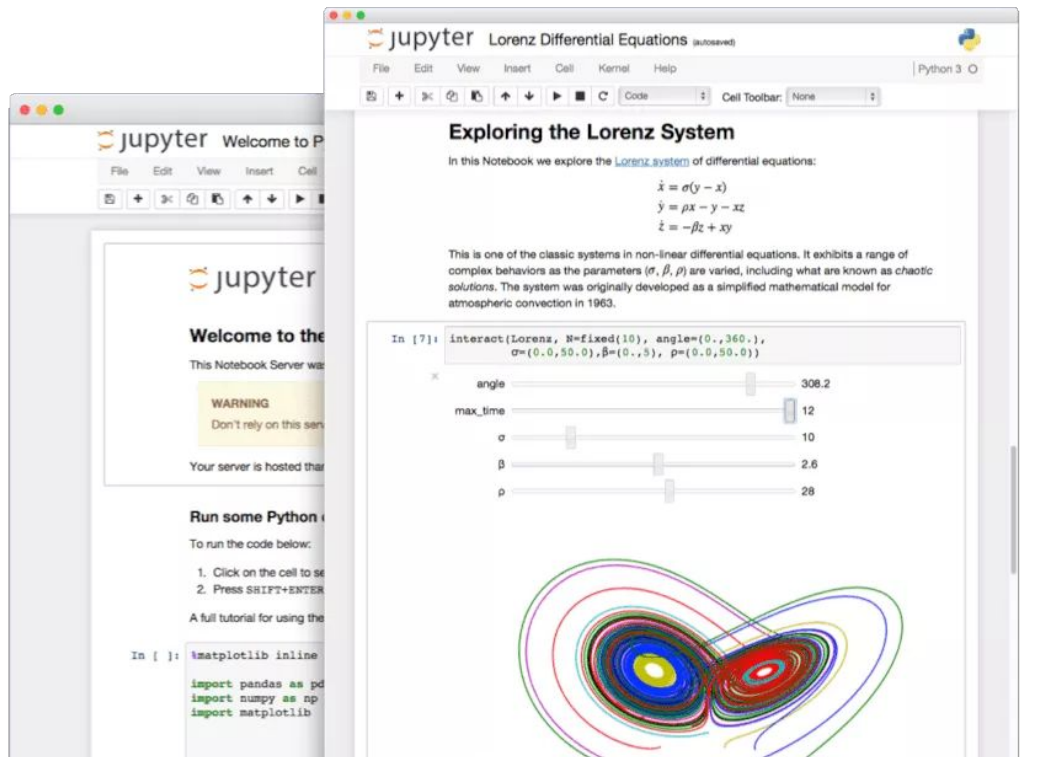
# Benefits

1. Scientists may already have an exploratory Jupyter Notebook
2. Jupyter Notebooks are easy for researchers to modify and maintain
3. Well-maintained widget ecosystem for visualization

# 1 Scientists may have an exploratory notebook

Jupyter is a web application for creating and sharing computational documents

- text
- code
- visual outputs



## 2 Jupyter Notebooks are easy to modify & maintain

- Easy Python; no traditional web development (HTML, CSS, etc.)
- Code is centrally located - no multiframe framework
- Traditional debugging available but not required

```
In [20]: def f(x):  
         print(x)  
         interact(f, x=10)
```



The image shows a Jupyter Notebook interface. The top part is a code cell with the following Python code:

```
In [20]: def f(x):  
         print(x)  
         interact(f, x=10)
```

Below the code cell, there is an interactive slider for the variable `x`. The slider has a range from 10 to 17, with a current value of 15. A mouse cursor is hovering over the slider handle.

### 3 ipywidget ecosystem for visualizations

#### ▼ Select Network Graph

Select a decay denominator

Module	Quality	p-value	Module	In Module	Index	Recovered	Query Genes
N005M00333	0.5316	1.39987e-09	28	8	0.4737	44.4444	Svm9G0004840, Svm2G0016240, Svm3G
N005M00547	0.3228	0.106147	10	1	0.6667	5.5556	Svm2G0034600
N005M00671	0.4361	0.00141364	10	5	0.7826	27.7778	SvmUn2G0001010, SvmUn2G0001690, S
N005M00774	0.2097	0.437413	8	1	0.7200	5.5556	Svm9G0005060
N005M02108	0.2933	0.113573	8	2	0.7500	11.1111	Svm3G0017990, Svm2G0004330
N005M03718	0.6077	0.0105353	4	4	1.0000	22.2222	SvmUn2G0001610, SvmCPG0000110, Sv

#### ► Export

#### ▼ Network Graph of Selected Module

(No module selected.)

visualize networks with ipycytoscape

### 3 ipywidget ecosystem for visualizations

Interactive maps with ipyleaflet

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# Deployments and supported features

1. Shared Storage
2. User Authentication & Group Managmenet
3. Repeating Components

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ template\_nbs /

Name	Last Modified
template_lib	2 days ago
00_welco...	2 days ago
01_overvie...	6 days ago
01_welcom...	19 hours ago
• 02_data.ip...	7 minutes ago
03_selecti...	16 hours ago
04_visualiz...	7 days ago
APP.ipynb	7 days ago
EXAMPLE_...	7 days ago
logger.ipynb	a month ago
notebook.i...	2 months ago
standalone...	7 days ago
Untitled.ip...	7 days ago

Launcher APP.ipynb Untitled.ipynb 02\_data.ipynb APP.ipynb

Code Python 3 (ipykernel) Render on Save

```
[ ]:
```

```
from nb.cfg import model, view, ctrl
```

```
# Start MVC objects (to trace into a module, set a breakpoint  
model.start() # Load data or prepare access to data  
view.start() # Build user interface (specify "log=True" whe  
ctrl.start() # Run the app
```

```
[ ]:
```

**How do RSEs use  
Jupyter to create a  
web application?**





- Hosted on Purdue's Geddes composable platform
- Kubernetes to scalably deploy sessions of the application

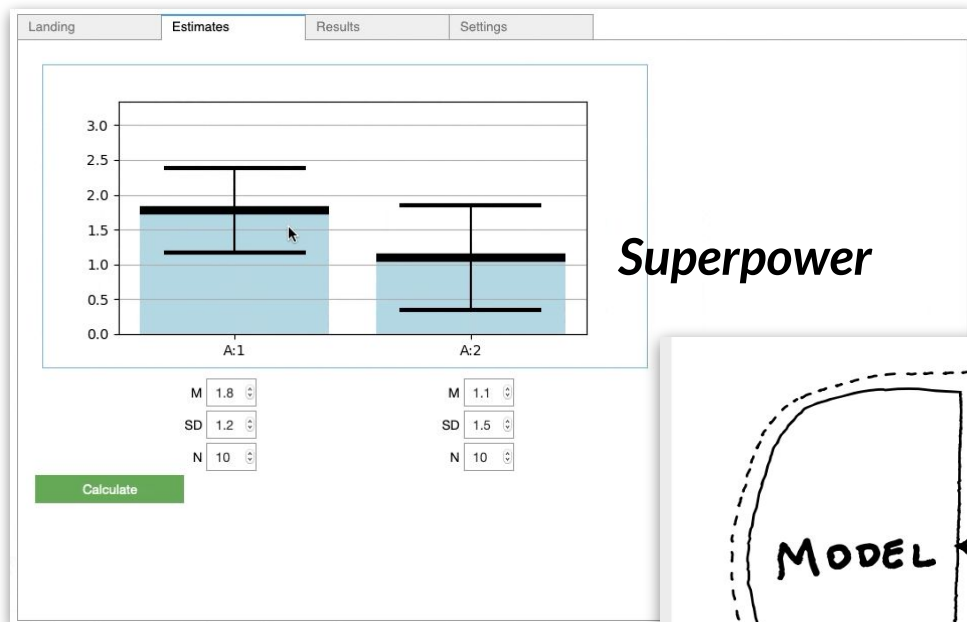


## 2 Authentication and Group Management



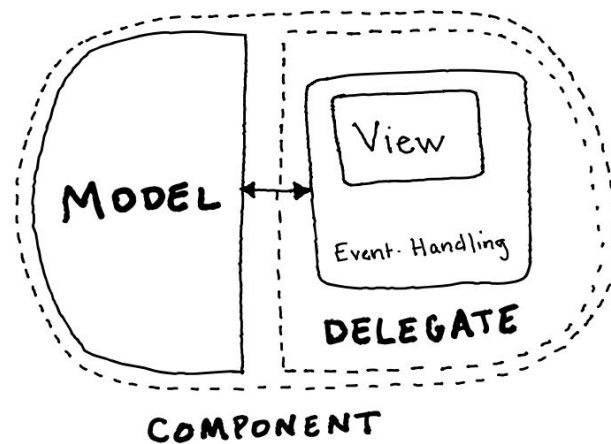
- Shared data storage among select users only
- Application hosted as a tool on MyGeoHub (science gateway built with HubZero)

### 3 Modularity and Interactive Plots



*Superpower*

- Repeating components
- Modified ModelDelegate design pattern for increased modularity
- Interactive plots with bidirectional communication



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# Limitations

- Limited stylistic control
- Widget ecosystem is largely built by third party developers
- Modularity requires OOP expertise
- Many data visualization libraries aren't interactive and may require custom JavaScript or other “hacky” solutions

# Review



Benefits	Supported Features	Limitations
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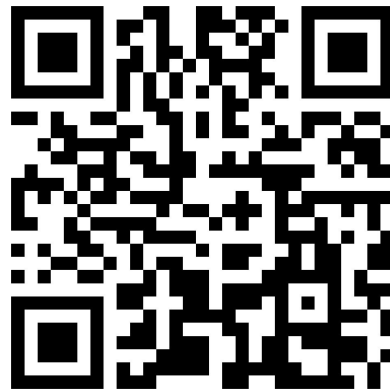
# Future work

- User groups not managed by science gateways
- Scalability
- Access to HPC resources
- Refactoring



## nicole-brewer/nbdev\_app\_template

- Dockerfile for deploying on a composable platform
- Docker-compose for development environment
- Extended version of the nbdev template with instructional notebooks and templates



Give the repo a  and watch for updates