

Running Jupyter Notebook and RStudio on Minerva

Minerva Scientific Computing Environment

<https://labs.icahn.mssm.edu/minervalab>

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What is a container?

- **Simply put, a container is a sandboxed process on your machine that is isolated from all other processes on the host machine. A container:**
 - Is a runnable instance of an image.
 - Can be run on local machines, virtual machines or deployed to the cloud.
 - Is portable (can be run on any OS).
 - Is isolated from other containers and runs its own software, binaries, and configurations.
- **Why use containers?**
 - Software developers can build their stack onto whatever operating system base fits their needs best, and create distributable runtime environments so that users never have to worry about dependencies and requirements, that they might not be able to satisfy on their systems.
- **More information:**
 - Docker: <https://docs.docker.com/get-started/>
 - **Singularity:** <https://docs.sylabs.io/guides/3.11/user-guide/introduction.html>
 - Minerva training sessions:
<https://labs.ica hn.mssm.edu/minervalab/resources/the-minerva-user-group-and-training-classes/>

Jupyter Notebook

The Jupyter Notebook is the original web application for creating and sharing computational documents. It offers a simple, streamlined, document-centric experience. (<https://jupyter.org/>)

The image displays two overlapping screenshots of a Jupyter Notebook interface. The background screenshot shows the 'Welcome to Jupyter' page, which includes a warning message and instructions on how to run Python code. The foreground screenshot shows a notebook titled 'Exploring the Lorenz System'. The notebook content includes the following text and code:

Exploring the Lorenz System

In this Notebook we explore the `Lorenz.system` of differential equations:

$$\begin{aligned}\dot{x} &= \sigma(y - x) \\ \dot{y} &= \rho x - y - xz \\ \dot{z} &= -\beta z + xy\end{aligned}$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of complex behaviors as the parameters (σ, β, ρ) are varied, including what are known as chaotic solutions. The system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

```
In [7]: interact(Lorenz, N=fixed(10), angle=(0.,360.),
                sigma=(0.0,50.0),beta=(0.,5), rho=(0.0,50.0))
```

The interactive widget shows sliders for the following parameters:

- angle: 308.2
- max_time: 12
- σ : 10
- β : 2.6
- ρ : 28

Below the widget is a 3D plot of the Lorenz attractor, showing its characteristic butterfly shape with multiple colored trajectories.

How to Run Jupyter Notebook on Minerva

Option 1 : On-the-fly Jupyter Notebook in a Minerva job

<https://labs.icaahn.mssm.edu/minervalab/documentation/python-and-jupyter-notebook/#jupyter>

- Scripts in /usr/local/bin on head nodes only:
 - `minerva-jupyter-web.sh`
 - Runs jupyter installed inside a singularity container
 - No module system setup
 - `minerva-jupyter-module-web.sh`
 - Runs jupyter installed in module python/3.7.3
 - Can access modules on minerva
 - Can load users' conda environments (jupyter must be installed in conda env)
- Add `--help` to the script to get help message/usage
- How to create conda environment on Minerva:

<https://labs.icaahn.mssm.edu/minervalab/documentation/conda/>

How to Run Jupyter Notebook on Minerva

Option 2 : Jupyter Notebook in a batch job

- Primarily, the nbconvert tool allows you to convert a Jupyter .ipynb notebook document file into another static format including HTML, LaTeX, PDF, Markdown, reStructuredText, and more. nbconvert can also add productivity to your workflow when used to execute notebooks programmatically.

<https://nbconvert.readthedocs.io/en/latest/usage.html>

- Use the commands below in your job script:

```
m1 python
```

```
    jupyter nbconvert --to notebook --execute myfile.ipynb
```

- The result is saved in a file named **myfile.nbconvert.ipynb**

How to Run RStudio on Minerva

Option 1 : On-the-fly Rstudio over Web in a Minerva job

<https://labs.icahn.mssm.edu/minervalab/documentation/r/#rstudio>

- Scripts in /usr/local/bin on head nodes only:
 - `minerva-rstudio-web-r4.sh`
 - ~~`minerva-rstudio-web-r4.2.1.sh`~~
 - `minerva-rstudio-web-r4.2.3.sh`
- All scripts run RStudio Server installed inside singularity containers
- No module system setup
- Add `--help` to the script to get help message/usage

Option 2 : Run rstudio over GUI (graphical user interface)

- Enable X11 forwarding
- Run `m1 rstudio proxies; rstudio`

Install R packages with On-the-fly RStudio over Web

```
minerva-rstudio-web-r4.sh -h
```

```
...
```

```
[INFO] === Package Installations ===
```

```
[INFO] To install R packages, do the following in the RStudio web *Shell terminal console*
```

```
[INFO] $ export http_proxy=http://172.28.7.1:3128
```

```
[INFO] $ export https_proxy=http://172.28.7.1:3128
```

```
[INFO] $ export all_proxy=http://172.28.7.1:3128
```

```
[INFO] $ export no_proxy=localhost,*.hpc.mssm.edu,*.chimera.hpc.mssm.edu,172.28.0.0/16
```

```
[INFO] $ R
```

```
[INFO] >>> install.packages(name_of_package)
```

```
[INFO] The packages will be installed in your
```

```
/hpc/users/yuj25/R/x86_64-pc-linux-gnu-library/R_VERSION
```

```
[INFO] If the package is not available in your RStudio Web interface by R
```

```
library('name_of_package')
```

```
[INFO] You can restart the RStudio job
```

```
...
```


RStudio Connect server <https://rstudio-connect.hpc.mssm.edu>

- You can publish Shiny, R Markdown for collaborators or others
- If interested in publishing on Rstudio-connect, please check instruction at <https://labs.icahn.mssm.edu/minervalab/documentation/r/#rstudioconnect>
 - Run “ml rstudio proxies firefox; rstudio” on a compute node
 - Shiny app example at <https://github.com/rstudio/shiny-examples>

Content / 012-datatables

Columns in diamonds to show:

- carat
- cut
- color
- clarity
- depth
- table
- price
- x
- y
- z

diamonds | mtcars | iris

Show 10 entries Search:

	carat	cut	color	clarity	depth	table	price
1	1.24	Premium	D	SI1	62.4	59	7486
2	1.2	Premium	G	VS2	62.1	61	7728
3	0.73	Very Good	F	SI1	59.7	60	2473
4	1.53	Premium	I	SI1	61.5	59	8911
5	0.3	Premium	D	SI1	62.1	59	515
6	0.58	Ideal	H	VS1	61.2	55	1671
7	0.51	Ideal	E	SI2	61	56	1098
8	1.5	Ideal	G	VVS2	61.3	56	17176
9	2.66	Good	H	SI2	63.8	57	16239
10	0.3	Premium	F	VVS2	61.4	59	737

Showing 1 to 10 of 1,000 entries

Previous **1** 2 3 4 5 ... 100 Next

Info Access Runtime Schedule Tags Vars Logs

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Lili Gai gail01

Add collaborator

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The default user rstudio-connect

Content URL

/hpcshowcase/

<https://rstudio-connect.hpc.mssm.edu> Copy

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CTSA Clinical & Translational[®]
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Last but not Least

- ▶ Got a problem? Need a program installed? Send an email to:

hpchelp@hpc.mssm.edu