

# Benefits and Perils of Open-Source Software



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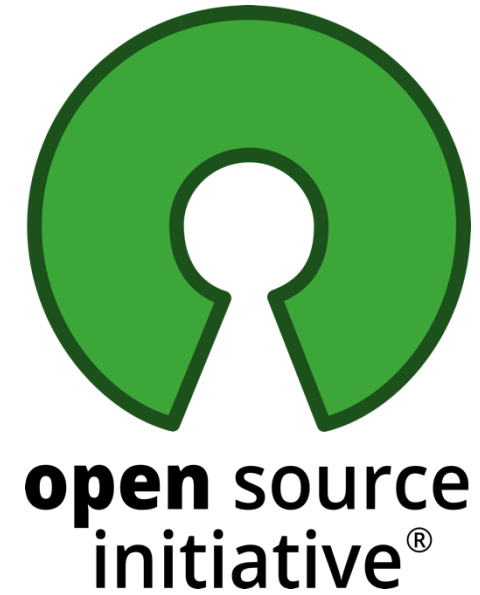
<https://github.com/Whitford/ctbp-techtalks>

**Vinícius Contessoto**

contessoto@rice.edu – Oct/2024

# Outline

- What is Open-Source Software (OSS)?
- History – Timeline - OSS
- Licenses
- Environments

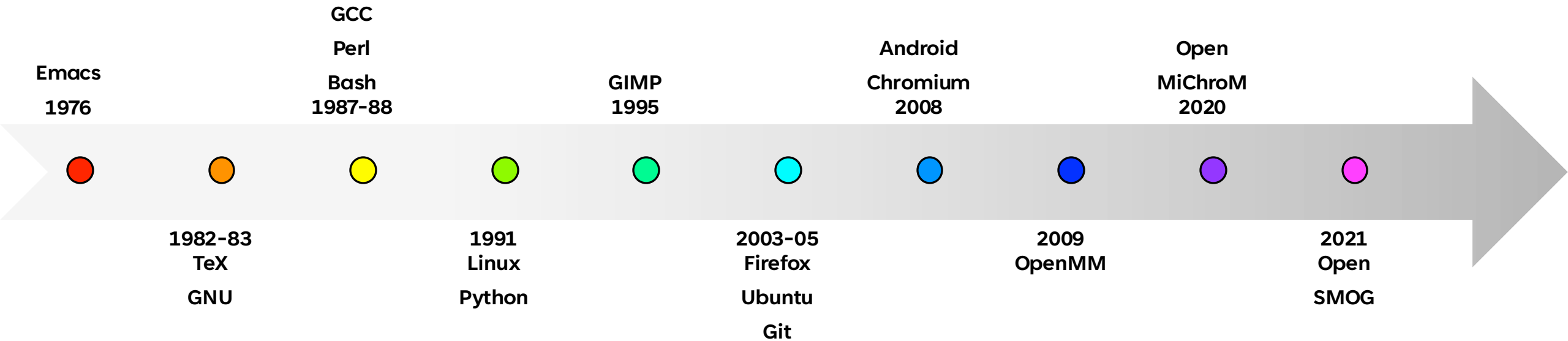


# Open-Source Software - OSS

**OSS** is computer software that is released under a **license** in which the **copyright holder** grants **users** the rights to **use, study, change, and distribute** the software and its source code to **anyone** and for any **purpose**.

**Collaboration + Scientific Community**

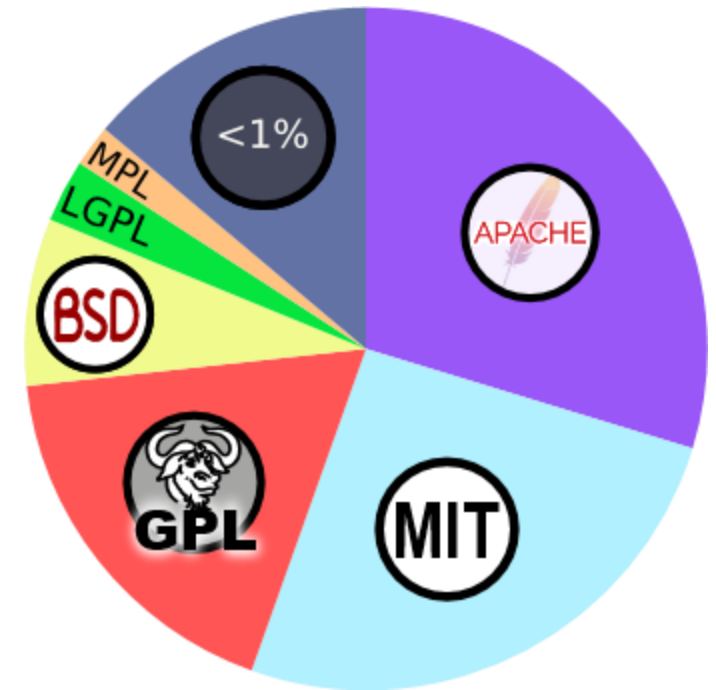
# Timeline



“Beware of bugs in the above code; I have only proved it correct, not tried it.” - Donald Knuth, 1977

# Licenses

- Apache License 2.0
- BSD 3-Clause and BSD 2-Clause Licenses
- All versions of the GPL
- All versions of the LGPL
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# OSS in Scientific Research

- Python Libraries:
  - NumPy: Numerical computing.
  - SciPy: Advanced scientific computations.
  - Matplotlib: Data visualization.
  - Pandas: Data manipulation and analysis.
  - Jupyter Notebook: Interactive computing environment.

# Example - Numpy

<https://numpy.org>



- Issues tracker - <https://github.com/numpy/numpy/issues>
- Ecosystem compatibility - <https://github.com/numpy/numpy/issues/26191>

“There is always a bug” - José Onuchic, 2017



# Managing Python Environments

- Avoid Versions conflicts
- Isolate your project dependencies
- Easier for collaboration and code sharing/deployment

# Managing Python Environments



```
> which python3 pip3
/opt/anaconda3/bin/python3
/opt/anaconda3/bin/pip3

> python3 --version
Python 3.11.8

> pip3 --version
pip 23.3.1 from /opt/anaconda3/lib/python3.11/site-packages/pip (python 3.11)

> mkdir tech_talks_2024
> cd tech_talks_2024/
```

# Managing Python Environments

```
● ● ●  
  
> python3 -m venv venv  
  
> ls  
venv  
  
> source venv/bin/activate  
  
> pip3 install numpy scipy opensmog  
  
> pip3 list  
Package      Version  
-----  
lxml         5.3.0  
numpy        2.1.2  
OpenSMOG     1.1.1  
pip          24.0  
scipy        1.14.1  
setuptools   65.5.0
```

# Managing Python Environments

```
● ● ●  
  
> pip3 freeze > requirements.txt  
  
> ls  
requirements.txt    venv  
  
> cat requirements.txt  
lxml==5.3.0  
numpy==2.1.2  
OpenSMOG==1.1.1  
scipy==1.14.1
```

# Managing Python Environments

```
● ● ●  
  
> deactivate  
  
> ls  
requirements.txt    venv  
  
> rm -rf venv  
  
> ls  
requirements.txt  
  
> python3 -m venv venv_new  
  
> source venv_new/bin/activate  
  
> pip3 list  
Package      Version  
-----  
pip          24.0  
setuptools   65.5.0
```

# Managing Python Environments

```

> > pip3 install -r requirements.txt

> pip3 list
Package      Version
-----
lxml          5.3.0
numpy         2.1.2
OpenSMOG      1.1.1
pip           24.0
scipy         1.14.1
setuptools    65.5.0

> pip3 install pipdeptree

> pipdeptree
OpenSMOG==1.1.1
├── lxml [required: Any, installed: 5.3.0]
└── numpy [required: Any, installed: 2.1.2]
pipdeptree==2.23.4
├── packaging [required: >=24.1, installed: 24.1]
└── pip [required: >=24.2, installed: 24.2]
scipy==1.14.1
└── numpy [required: >=1.23.5,<2.3, installed: 2.1.2]
setuptools==65.5.0
```

# CTBP – Resources & Useful links

- <https://kb.rice.edu/page.php?id=108237> (**NOTS**)
- <https://wiki.rice.edu/confluence/display/CTBP/CTBP+Computing+Activities> (**CTBP**)
- <https://researchcomputing.rice.edu> (**CRC**)
- <https://slurm.schedmd.com/tutorials.html> (**SLURM**)

