

# Containers, Singularity & Pitágoras

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# Outline

**Disclaimer:** esta apresentação representa apenas a experiência e opinião dos seus autores.

- Context: sharing a dashboard
- Containers: realçar o contexto de data science
- Pitágoras
- Singularity
  - Definition file
  - Build a container
  - Using the container in Pitágoras' platform
- Take-away

# Example: share a dashboard

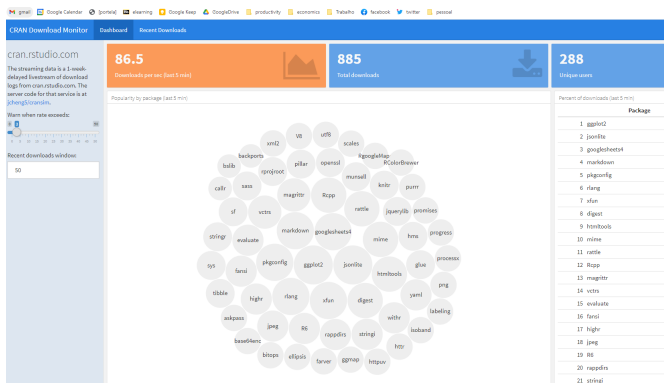


Figure 1: Flexdashboard example.

# Containers

- Package code and all its dependencies
- Lightweight and standardized piece of software  
Summarized by a definition file or image, which can be executed across many platforms
- Ideal solution to share a tool targetting a specific problem at hand
- Docker and Singularity are among the most used container systems
- Singularity images are particularly suited for data processing
- Outperforms Docker in access to host filesystem, networking, GPU computation, and security integration while optimizing reproducibility

# Containers

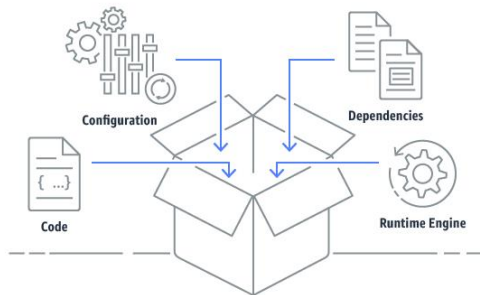
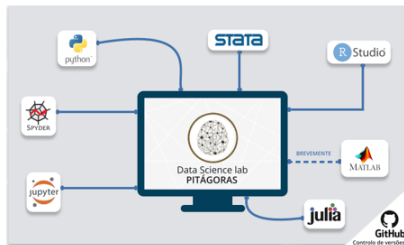


Figure 2: Container diagram

## Modern Data Architecture - Data Science Lab

- Grid computing solution
- Containerized and customizable runtimes and IDE's (singularity containers)
- Dedicated storage
- Batch executions
- Interactive executions (IDE's, Notebooks, etc.)
- + GitHub Enterprise Server



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Figure 3: Pitágoras environment. © Guilherme de Sousa.

# Pitágoras

- How to get there

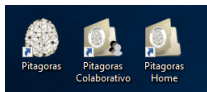


Figure 4: Pitágoras' icons.

- Sharing files with Pitágoras' infrastructure

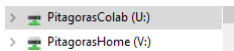
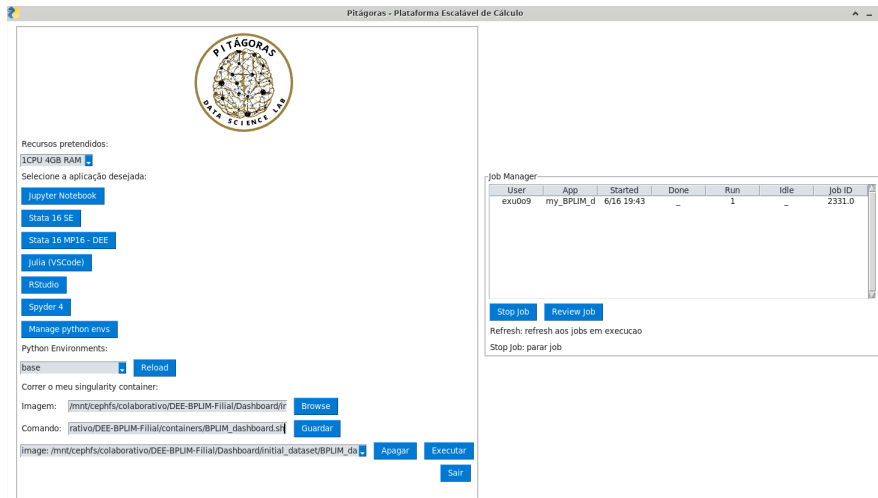


Figure 5: Pitágoras' icons.

# Using Pitágoras: GUI



The screenshot displays the Pitágoras GUI with the following sections:

- Header:** Pitágoras - Plataforma Escalável de Cálculo
- Logo:** A circular logo with a brain-like network structure, labeled "PITÁGORAS" and "DATA SCIENCE LAB".
- Recursos pretendidos:** A dropdown menu showing "1CPU 4GB RAM".
- Selecione a aplicação desejada:** A list of application buttons: Jupyter Notebook, Stata 16 SE, Stata 16 MP16 - DEE, Julia (VSCode), RStudio, Spyder 4, and Manage python envs.
- Python Environments:** A dropdown menu showing "base" and a "Reload" button.
- Correr o meu singularity container:** Fields for "Imagem:" (containing "/mnt/cephfs/colaborativo/DEE-BPLIM-Filial/Dashboard/ir") and "Comando:" (containing "rativo/DEE-BPLIM-Filial/containers/BPLIM\_dashboard.sh"), each with a "Browse" or "Guardar" button respectively.
- Buttons:** "Apagar", "Executar", and "Sair" buttons at the bottom.
- Job Manager:** A table showing job status and controls.

| User   | App        | Started    | Done | Run | Idle | Job ID |
|--------|------------|------------|------|-----|------|--------|
| exu0o9 | my_BPLIM_d | 6/16 19:43 | -    | 1   | -    | 2331.0 |

Below the Job Manager table are buttons for "Stop job" and "Review job".

Refresh: refresh aos jobs em execucao  
Stop job: parar job

Figure 6: Pitágoras' Graphical User Interface.



# Using Singularity in Pitágoras

- Go to Applications and open the 'Terminal Emulator'

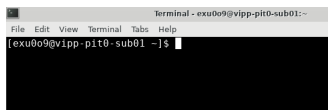


Figure 7: Pitágoras' terminal [@vipp].

- Move to folder  
/mnt/cephfs/colaborativo/SHARED-FOLDER
- Run the following two lines

```
export https_proxy=http://USER:  
password@proxy.bportugal.pt:8080
```

```
export http_proxy=http://USER:  
password@proxy.bportugal.pt:8080
```

# Using Singularity

## Singularity bit-by-bit

- Build a container

```
singularity build --fakeroot bplim_v0.sif  
bplim_v0.def
```

- Connect to the infrastructure

```
condor_submit -i
```

- Launch the container

```
singularity shell bplim.sif
```

- Use Jupyter Lab inside the container

```
jupyter lab
```

# Take-away

- Identify which tasks should be containerized
- Define the minimal setup you need for the container
- Practice

# Links

- Pitágoras: `pitagoras-wiki.bportugal.pt`
- Singularity, Definition files: `https://sylabs.io/guides/3.7/user-guide/definition\_files.html`
- Sylabs: `https://cloud.sylabs.io/home`
- SingularityHub: `https://singularityhub.github.io/`
- Jupyter: `https://jupyter.org/`

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