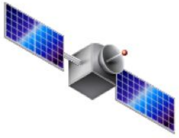
Rosetta



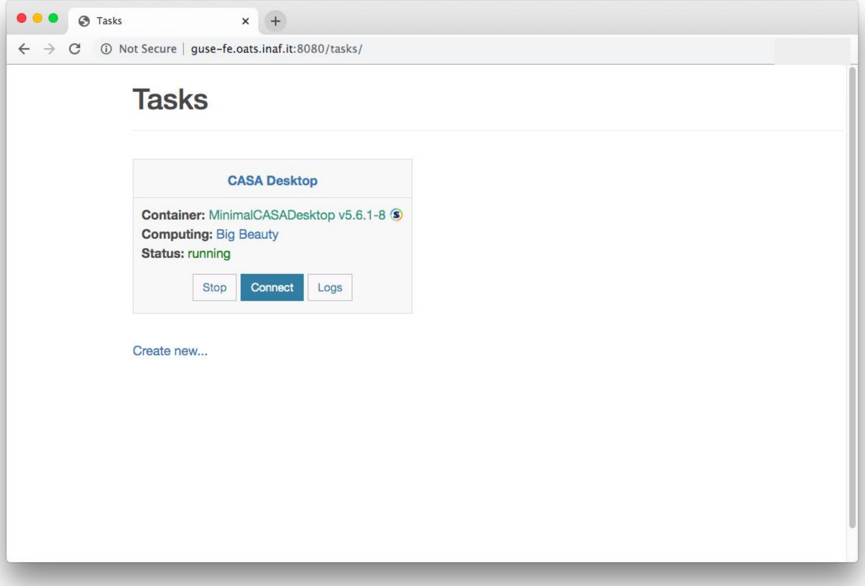
A container-centric science platform for interactive workloads

Rosetta in a nutshell

- Web-based science platform supporting GUI-based, interactive computing
- Batteries included, runs entirely on Docker containers
- Executes workloads in Docker or Singularity containers on a number of computing elements:
    - local CPUs;
    - remote servers (including commercial Clouds);
    - HPC Clusters (i.e. Slurm).
- Requires minimum effort to get Rosetta-compatible (just extend base containers)
- Allows users to setup and run their own containers, autonomously.

Example

- Task list and remote desktop container connection via automatic tunneling and Web VNC

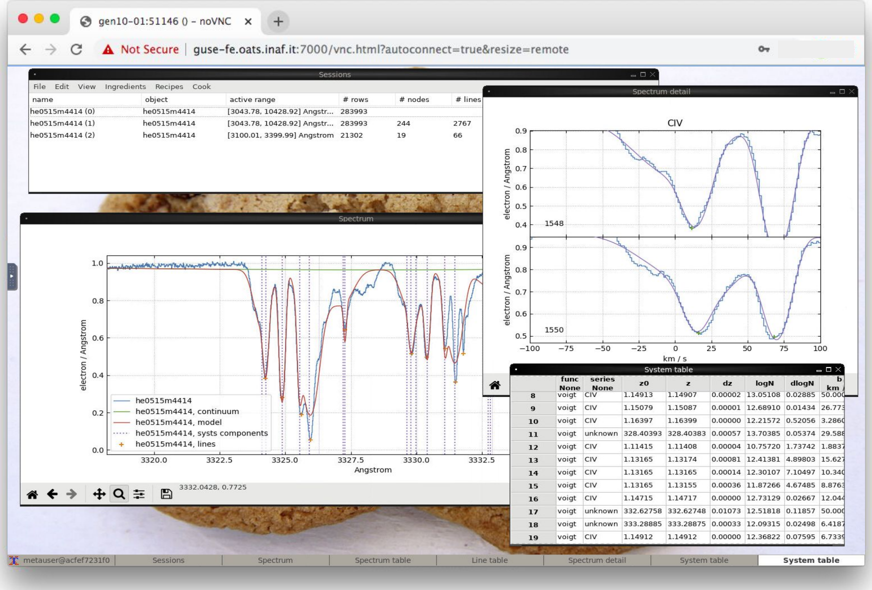


Tasks

CASA Desktop

Container: MinimalCASADesktop v5.6.1-8
Computing: Big Beauty
Status: running

Create new...



name	object	active range	# rows	# nodes	# lines
he0515m4414 (0)	he0515m4414	[3043.78, 10428.92] Angstr...	283993		
he0515m4414 (1)	he0515m4414	[3043.78, 10428.92] Angstr...	283993	244	2767
he0515m4414 (2)	he0515m4414	[3100.01, 3399.99] Angstrom	21302	19	66

	func None	series None	z0	z	dz	logN	dlogN	b km /
8	voigt	CIV	1.14913	1.14907	0.00002	13.05108	0.02885	50.000
9	voigt	CIV	1.15079	1.15087	0.00001	12.68910	0.01434	26.773
10	voigt	CIV	1.16397	1.16399	0.00000	12.21572	0.52056	3.2860
11	voigt	unknown	328.40393	328.40383	0.00057	13.70385	0.05374	29.588
12	voigt	CIV	1.11415	1.11408	0.00004	10.75720	1.73742	1.8837
13	voigt	CIV	1.13165	1.13174	0.00081	12.41381	4.89803	15.627
14	voigt	CIV	1.13165	1.13165	0.00014	12.30107	7.10497	10.340
15	voigt	CIV	1.13165	1.13155	0.00036	11.87266	4.67485	8.8763
16	voigt	CIV	1.14715	1.14717	0.00000	12.73129	0.02667	12.044
17	voigt	unknown	332.62758	332.62748	0.01073	12.51818	0.11857	50.000
18	voigt	unknown	333.28885	333.28875	0.00033	12.09315	0.02498	6.4187
19	voigt	CIV	1.14912	1.14912	0.00000	12.36822	0.07595	6.7339

A step back: what container actually are?

> “Containers are a solution to the problem of how to get software to run reliably when moved from one computing environment to another.”

cio.com

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> “Containers are a solution to the problem of how to get software to run reliably when moved from one computing environment to another.”

cio.com

↓

A.K.A. the dependency hell problem

The “dependency hell” problem

Mike wants to use a new software.

Mike cannot find a precompiled version that works with his OS and/or libraries.

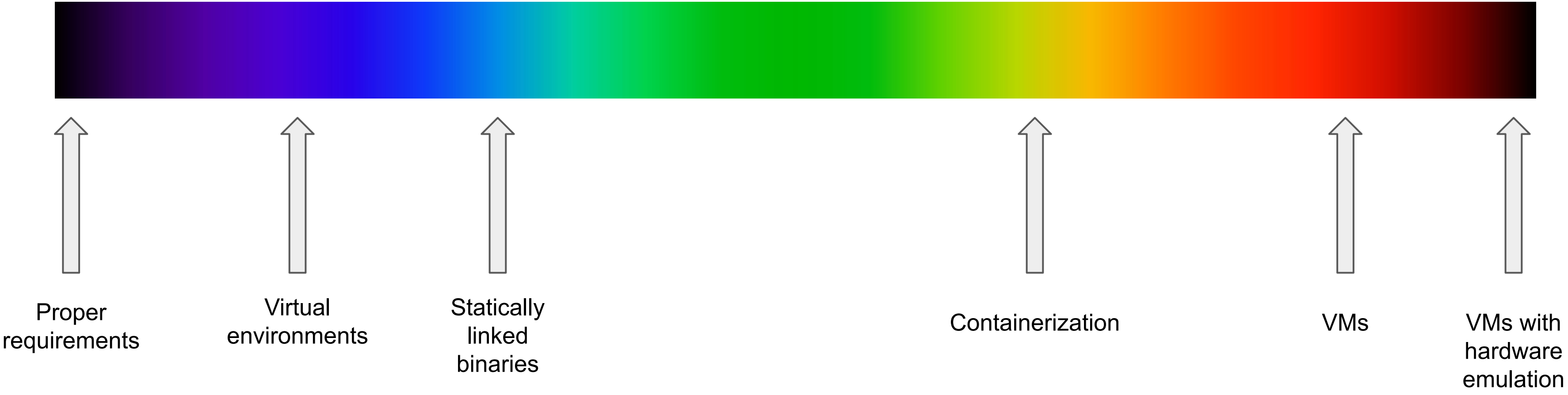
Mike asks/Google for help and gets some basic instructions - like “compile it”.

Mike starts downloading all the development environment, and soon realizes that he needs to upgrade (or downgrade!) some parts of his main Operating Systems.

During this process, something goes wrong.

Mikes spends an afternoon fixing his own OS, and all the next day in trying to compile the software. Which at the end turns out not to do what he wanted.

The “dependency hell” problem: solutions spectrum



Proper requirements

Virtual environments

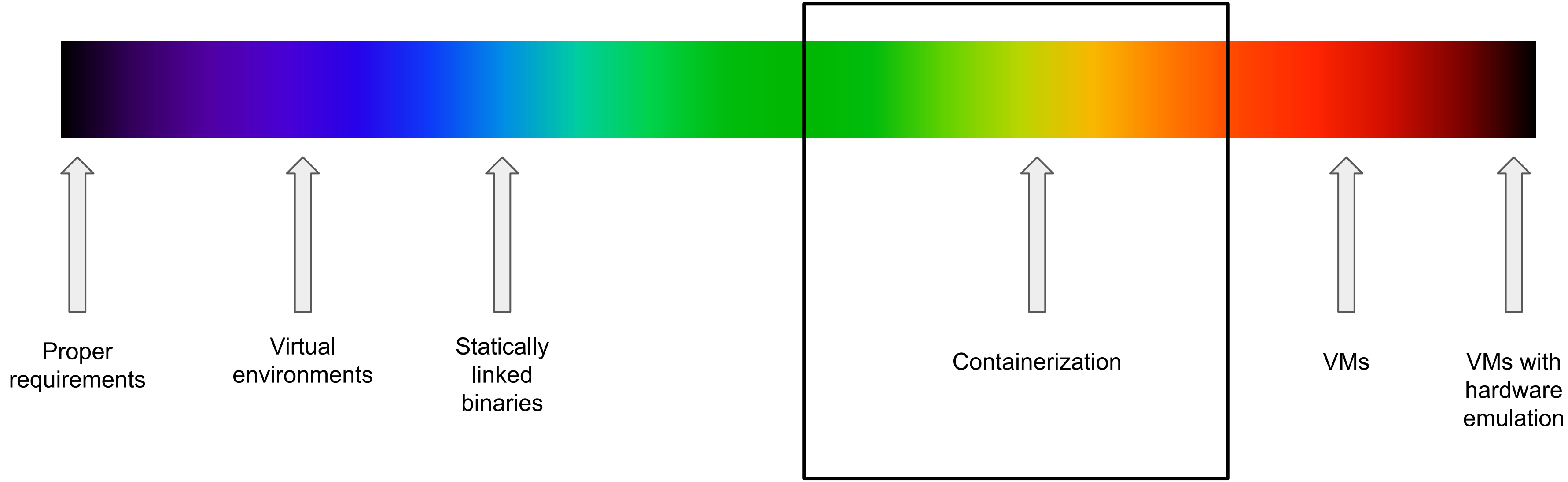
Statically linked binaries

Containerization

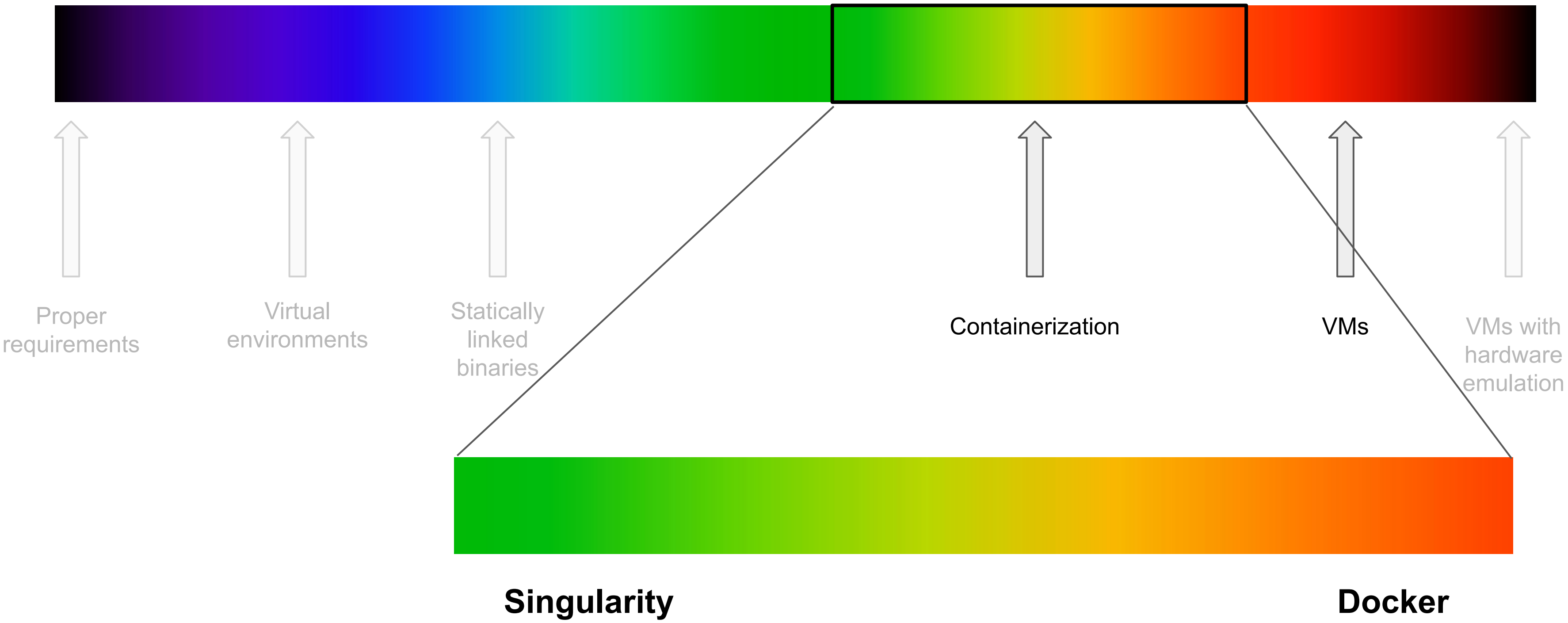
VMs

VMs with hardware emulation

The “dependency hell” problem: solutions spectrum



The “dependency hell” problem: solutions spectrum



Singularity vs Docker

Singularity	**Docker**
Scientific computing	IT industry standard
Running container are seen as processes	Running containers are seen as (micro)services
Build as root, run as user	Need near-root access or proper orchestrators
Limited or no support for networking	Extensive support for networking

Singularity vs Docker

Singularity	Docker
Filesystem: only partially isolated,directories as $HOME, /tmp, /proc, /sys, and /dev are all binded by default.	**Filesystem:** completely isolated by default, volume or folder binds must be explicitly set
Environment: from the host	**Environment:** from scratch
Network: from the host	**Network:** dedicated subnet

More similar to an environment

More similar to a virtual machine

Hard truth:

Environments-like containerisation solutions like Singularity do not not solve the dependency hell problem and how to reliably move software around, which in turn **does not guarantee reproducibility**!!

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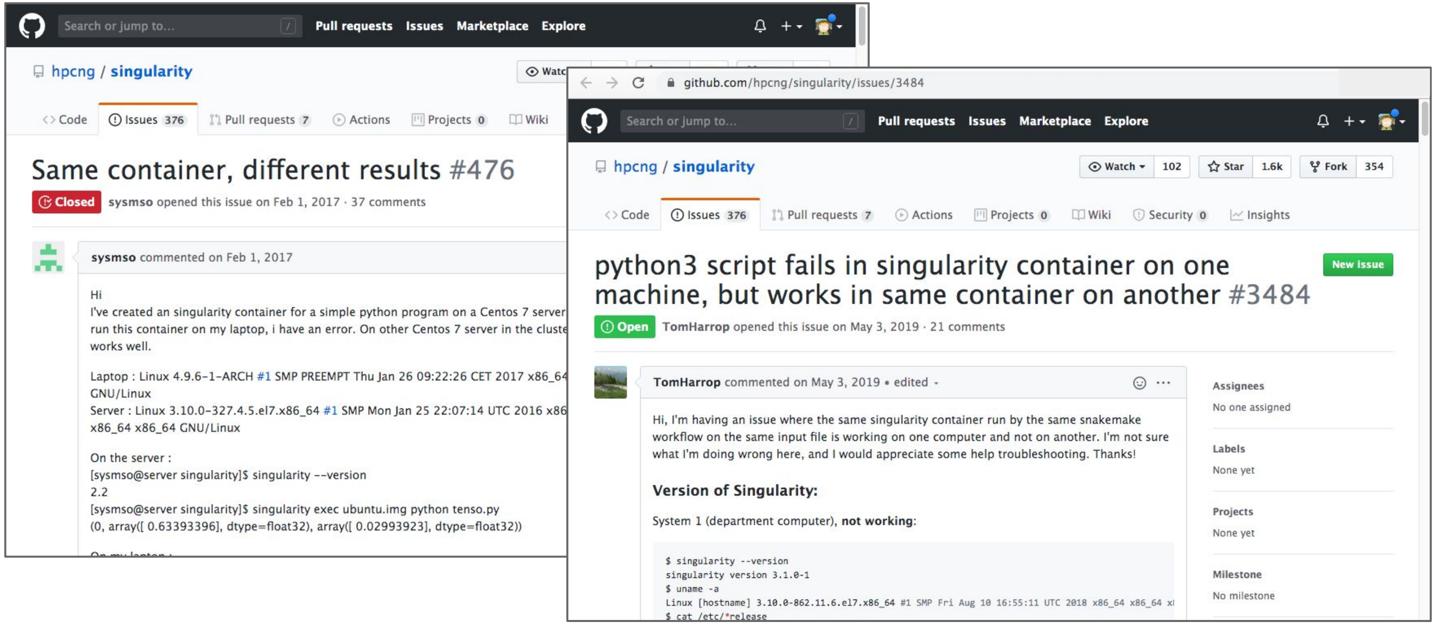


Same container, different results #476

Closed · **sysmso** opened this issue on Feb 1, 2017 · 37 comments

sysmso commented on Feb 1, 2017

Hi
I've created an singularity container for a simple python program on a Centos 7 server
run this container on my laptop, i have an error. On other Centos 7 server in the cluste
works well.

Laptop : Linux 4.9.6-1-ARCH #1 SMP PREEMPT Thu Jan 26 09:22:26 CET 2017 x86_64
GNU/Linux
Server : Linux 3.10.0-327.4.5.el7.x86_64 #1 SMP Mon Jan 25 22:07:14 UTC 2016 x86
x86_64 x86_64 GNU/Linux

On the server :

```
[sysmso@server singularity]$ singularity --version
2.2
[sysmso@server singularity]$ singularity exec ubuntu.img python tenso.py
(0, array([ 0.63393396], dtype=float32), array([ 0.02993923], dtype=float32))
```

python3 script fails in singularity container on one machine, but works in same container on another #3484

Open · **TomHarrop** opened this issue on May 3, 2019 · 21 comments

TomHarrop commented on May 3, 2019 • edited

Hi, I'm having an issue where the same singularity container run by the same snakemake workflow on the same input file is working on one computer and not on another. I'm not sure what I'm doing wrong here, and I would appreciate some help troubleshooting. Thanks!

Version of Singularity:

System 1 (department computer), **not working**:

```
$ singularity --version
singularity version 3.1.0-1
$ uname -a
Linux [hostname] 3.10.0-862.11.6.el7.x86_64 #1 SMP Fri Aug 10 16:55:11 UTC 2018 x86_64 x86_64 x
$ cat /etc/*release
```

Assignees
No one assigned

Labels
None yet

Projects
None yet

Milestone
No milestone

Singularity in Rosetta

Singularity is still very interesting as it can be used autonomously by users without asking much effort from sysadmins or to change the scheduling / workload management.

To overcome its environment-like limitations, in Rosetta Singularity is always forced to run in a specific way which allow to achieve an almost container-like behaviors, as Docker.

This requires a few specific command line switched (set by Rosetta itself) and some extra orchestration (for sandboxing)

```
mkdir -p /tmp/ee3f2776-1b9e-4dd4-a250-f80813dc9fe0_data/tmp && \
mkdir -p /tmp/ee3f2776-1b9e-4dd4-a250-f80813dc9fe0_data/home && \
chmod 700 /tmp/ee3f2776-1b9e-4dd4-a250-f80813dc9fe0_data && \
singularity run --pid --no-home --containall --cleanenv --writable-tmpfs
--workdir /tmp/ee3f2776-1b9e-4dd4-a250-f80813dc9fe0_data/tmp --home=/home/metauser \
-B/tmp/ee3f2776-1b9e-4dd4-a250-f80813dc9fe0_data/home:/home/metauser
```

Container interfaces & graphical applications

One missing bit in using containers (regardless of Docker or Singularity) is that the software you use to interact with your container ***is*** a dependency.

Usually, this dependency is a command-line, or a terminal, which is stable from the 80's.

However, with GUI applications, how to ensure the most common possible dependency?

Container interfaces & graphical applications

Possible options:

1. X11
2. VNC
3. Web-based VNC

Container interfaces & graphical applications

Possible options:

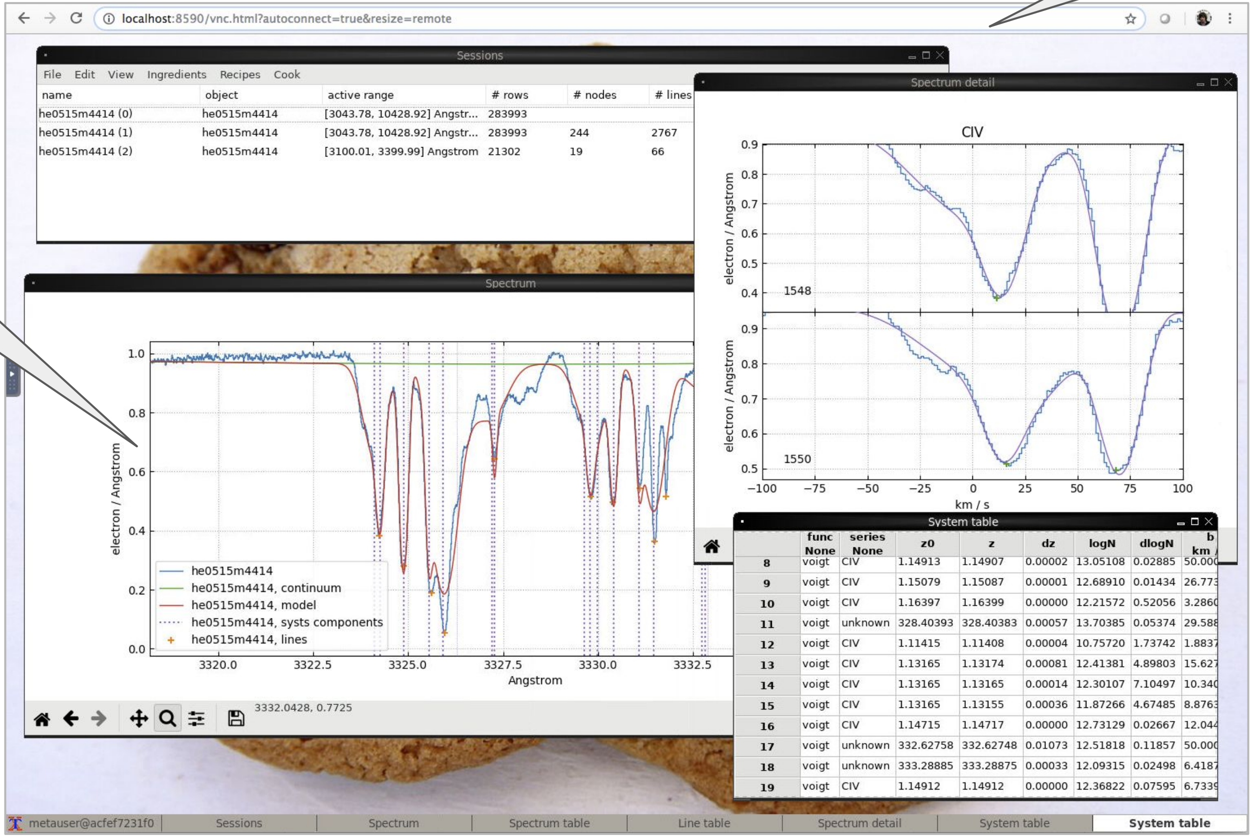
1. X11
2. VNC
3. Web-based VNC

This one. Why? ..because like it or not, web browsers and Javascript are the most standard technologies you can find in your usebase

..therefore:

The interface is the web browser

Reproducible scientific stuff within Singularity



localhost:8590/vnc.html?autoconnect=true&resize=remote

name	object	active range	# rows	# nodes	# lines
he0515m4414 (0)	he0515m4414	[3043.78, 10428.92] Angstr...	283993		
he0515m4414 (1)	he0515m4414	[3043.78, 10428.92] Angstr...	283993	244	2767
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14	voigt	CIV	1.13165	1.13165	0.00014	12.30107	7.10497	10.340
15	voigt	CIV	1.13165	1.13155	0.00036	11.87266	4.67485	8.8763
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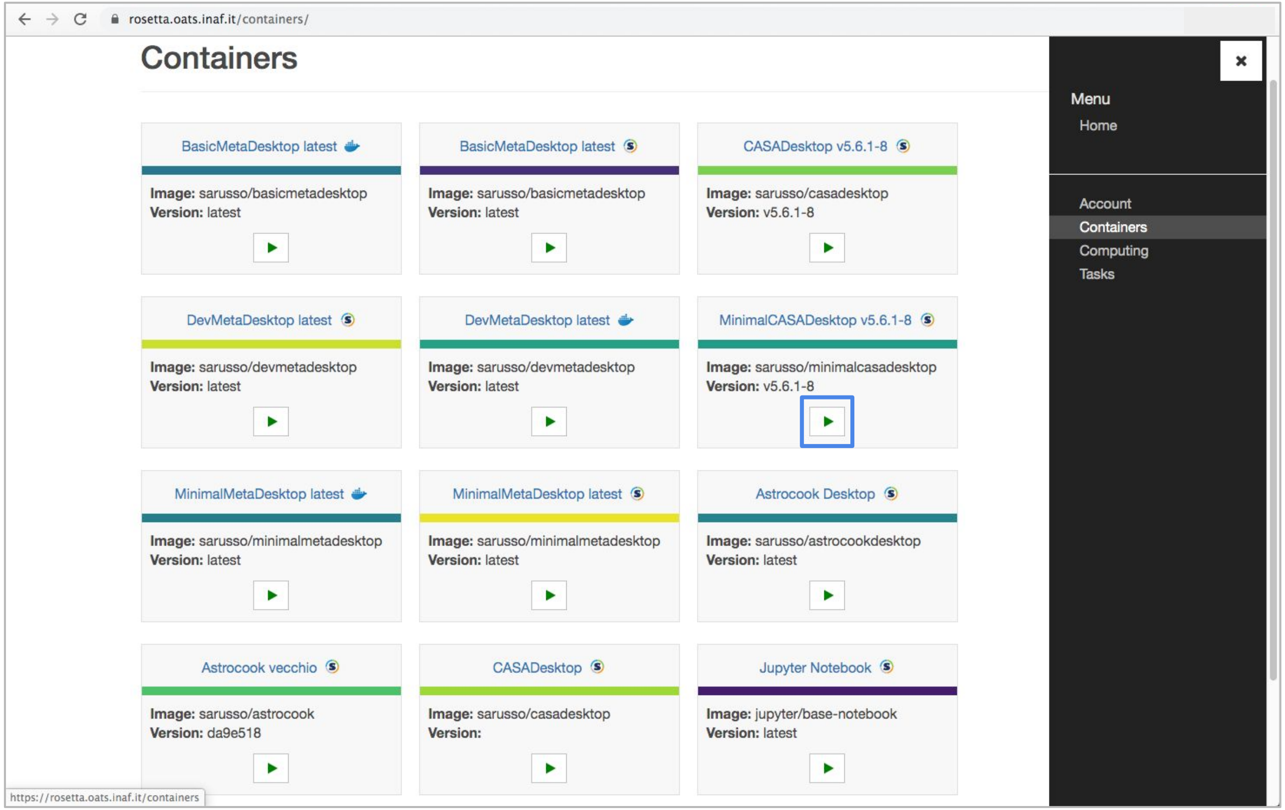
19	voigt	CIV	1.14912	1.14912	0.00000	12.36822	0.07595	6.7339

Rosetta quickstart & demo (for users)



rosetta.oats.inaf.it/containers/
Menu
Home
Account
Containers
Computing
Tasks
https://rosetta.oats.inaf.it/containers

Containers

BasicMetaDesktop latest
Image: sarusso/basicmetadesktop
Version: latest

BasicMetaDesktop latest
Image: sarusso/basicmetadesktop
Version: latest

CASADesktop v5.6.1-8
Image: sarusso/casadesktop
Version: v5.6.1-8

DevMetaDesktop latest
Image: sarusso/devmetadesktop
Version: latest

DevMetaDesktop latest
Image: sarusso/devmetadesktop
Version: latest

MinimalCASADesktop v5.6.1-8
Image: sarusso/minimalcasadesktop
Version: v5.6.1-8

MinimalMetaDesktop latest
Image: sarusso/minimalmetadesktop
Version: latest

MinimalMetaDesktop latest
Image: sarusso/minimalmetadesktop
Version: latest

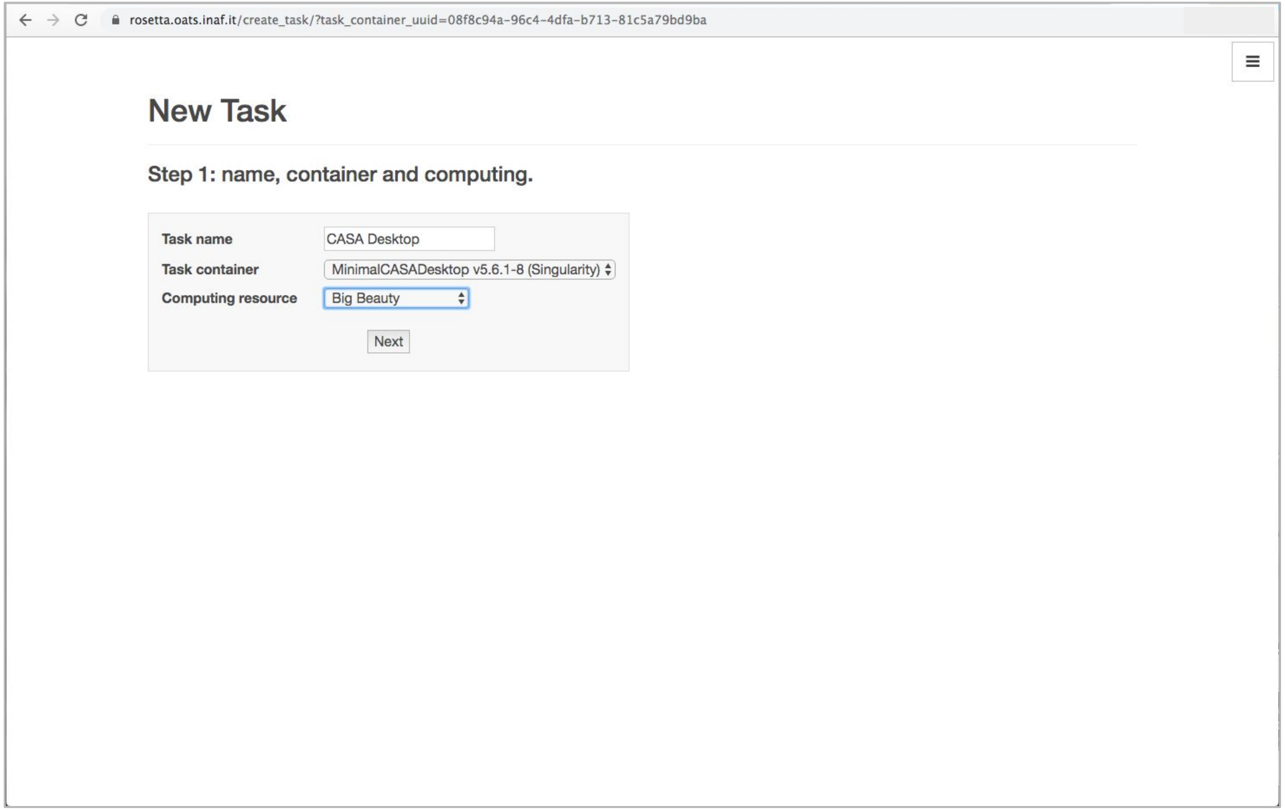
Astrocook Desktop
Image: sarusso/astrocookdesktop
Version: latest

Astrocook vecchio
Image: sarusso/astrocook
Version: da9e518

CASADesktop
Image: sarusso/casadesktop
Version:

Jupyter Notebook
Image: jupyter/base-notebook
Version: latest

Rosetta quickstart & demo (for users)



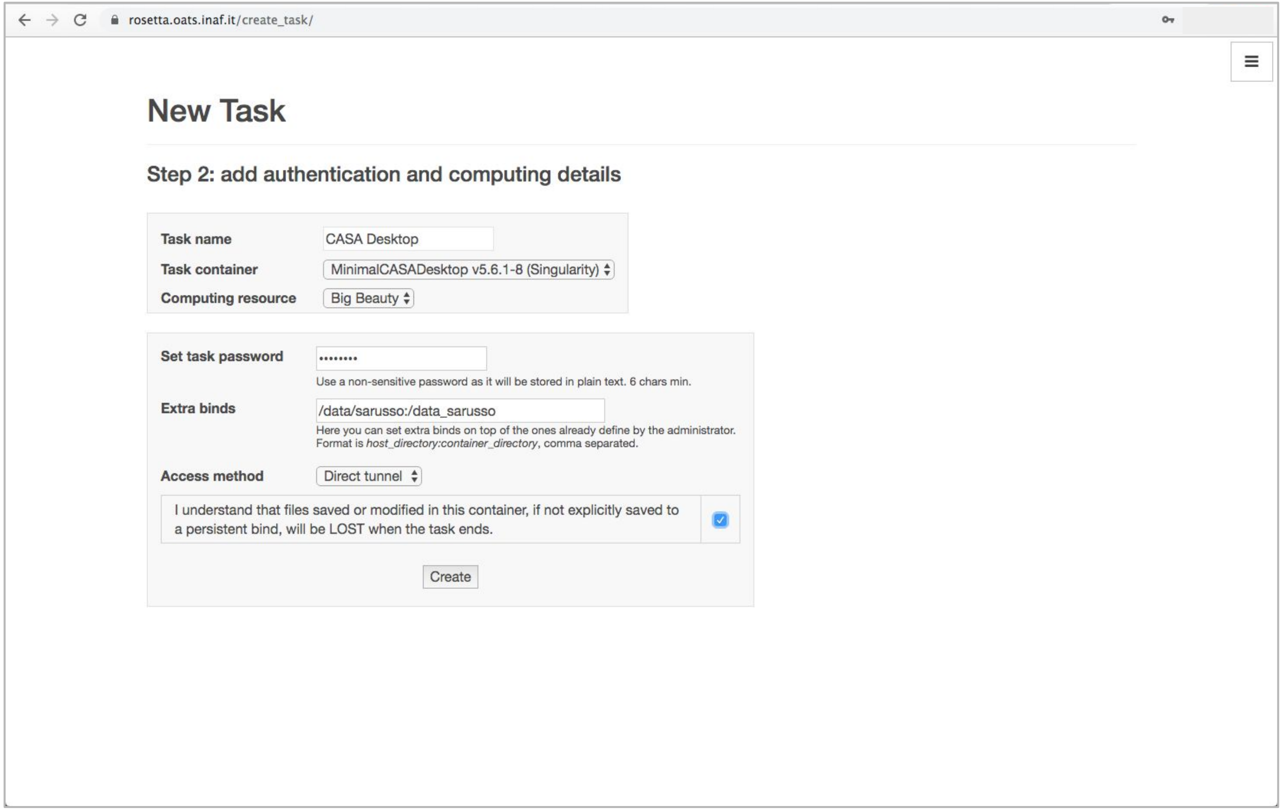
rosetta.oats.inaf.it/create_task/?task_container_uuid=08f8c94a-96c4-4dfa-b713-81c5a79bd9ba

New Task

Step 1: name, container and computing.

Task name	CASA Desktop
Task container	MinimalCASADesktop v5.6.1-8 (Singularity)
Computing resource	Big Beauty

Rosetta quickstart & demo (for users)



New Task

Step 2: add authentication and computing details

Task name	CASA Desktop
Task container	MinimalCASADesktop v5.6.1-8 (Singularity)
Computing resource	Big Beauty

Set task password ••••••••

Use a non-sensitive password as it will be stored in plain text. 6 chars min.

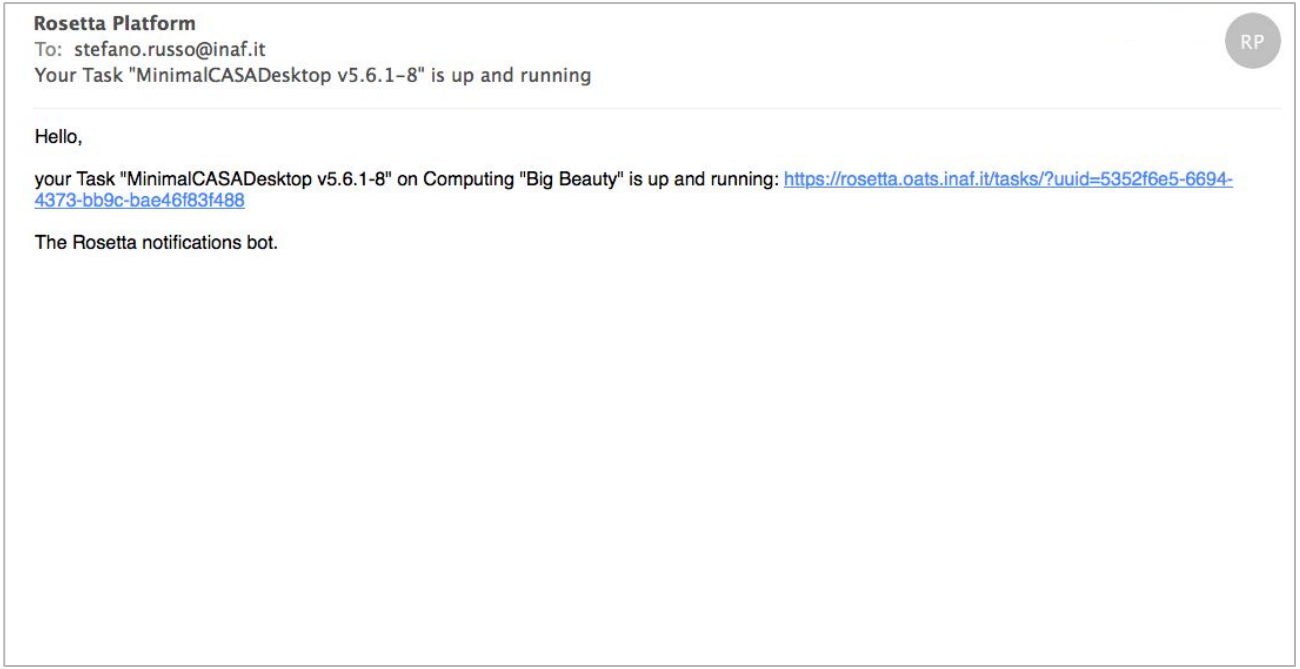
Extra binds /data/sarusso:/data_sarusso

Here you can set extra binds on top of the ones already define by the administrator. Format is *host_directory:container_directory*, comma separated.

Access method Direct tunnel

I understand that files saved or modified in this container, if not explicitly saved to a persistent bind, will be LOST when the task ends. ☑

Rosetta quickstart & demo (for users)



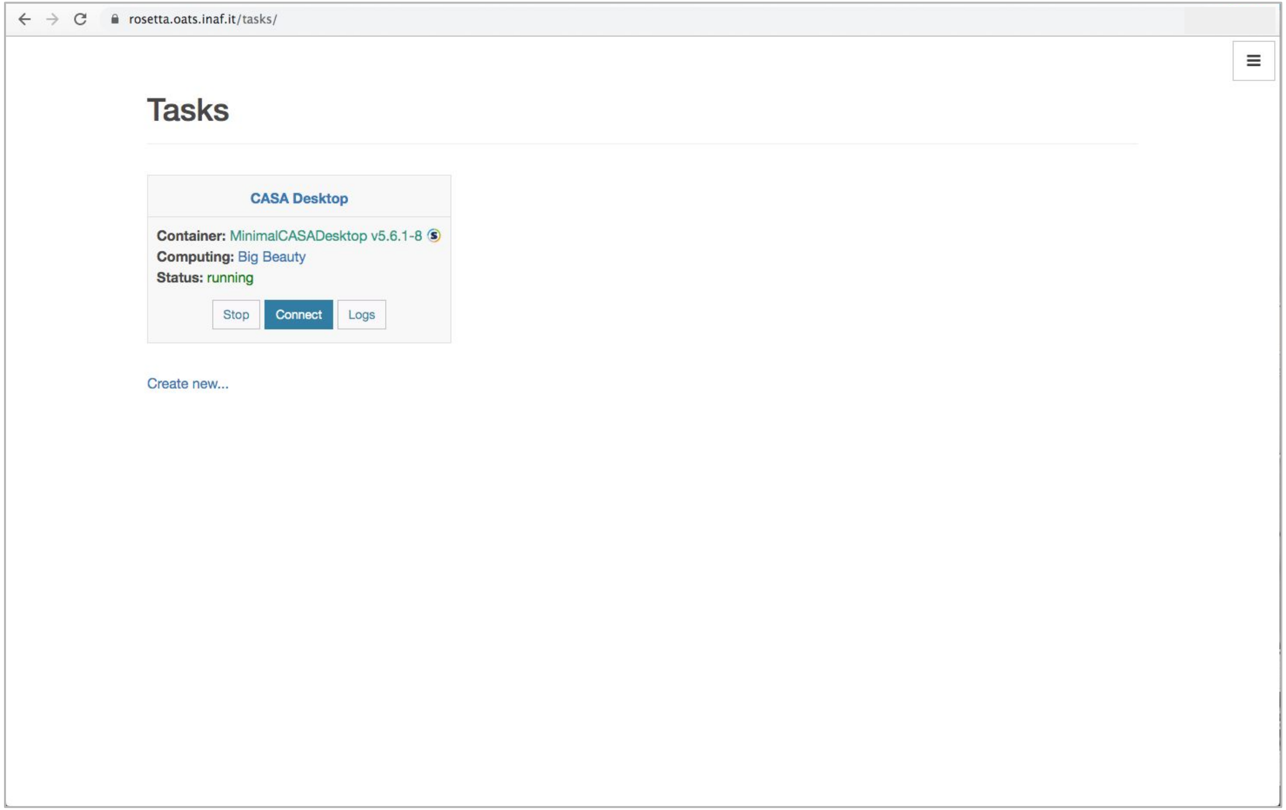
Rosetta Platform
To: stefano.russo@inaf.it
Your Task "MinimalCASADesktop v5.6.1-8" is up and running

Hello,

your Task "MinimalCASADesktop v5.6.1-8" on Computing "Big Beauty" is up and running: https://rosetta.oats.inaf.it/tasks/?uuid=5352f6e5-6694-4373-bb9c-bae46f83f488

The Rosetta notifications bot.

Rosetta quickstart & demo (for users)



Tasks

CASA Desktop

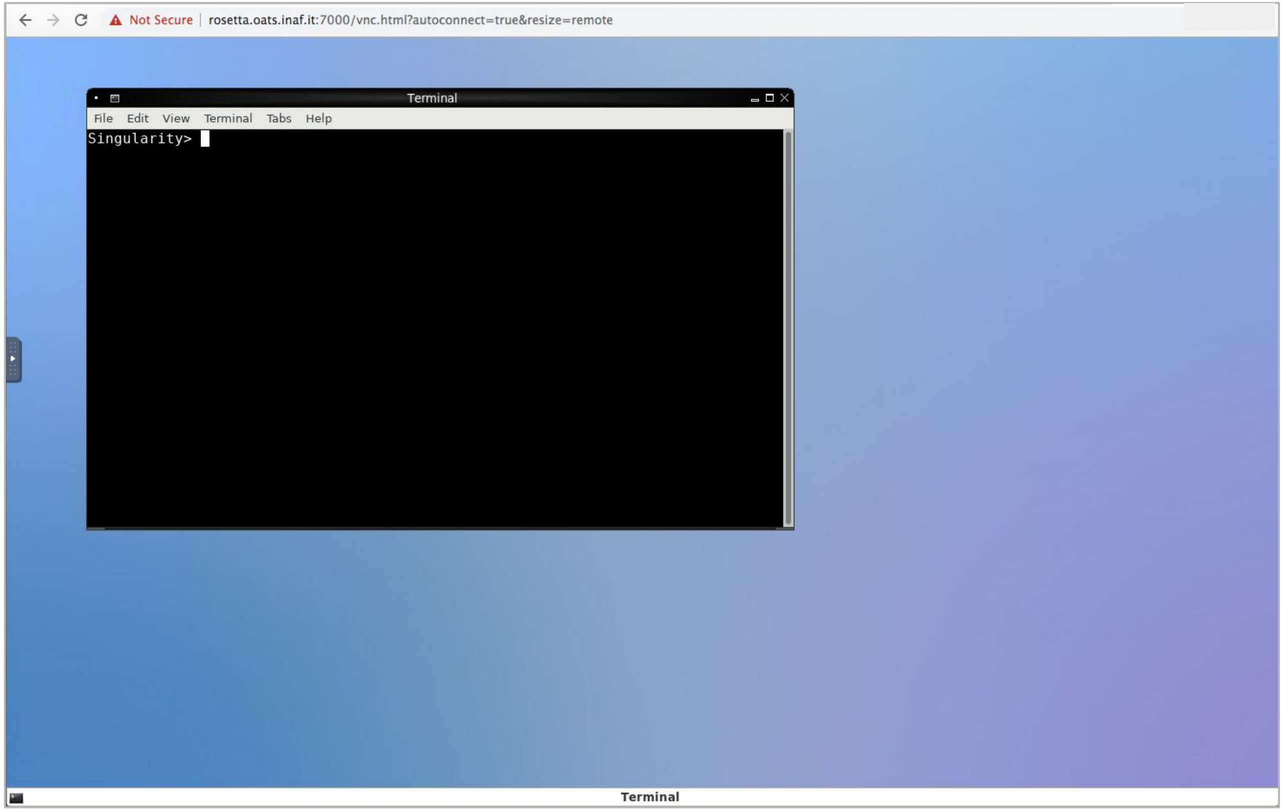
Container: MinimalCASADesktop v5.6.1-8

Computing: Big Beauty

Status: running

Create new...

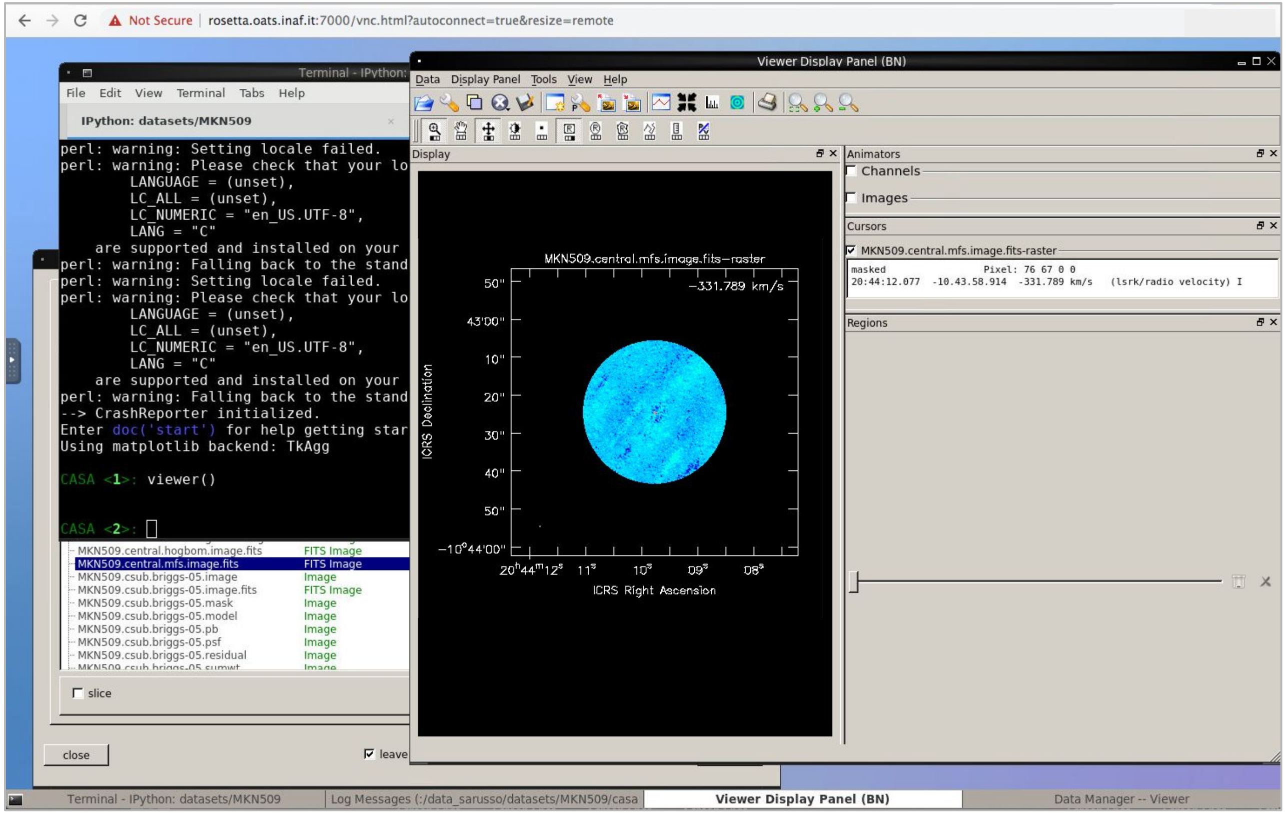
Rosetta quickstart & demo (for users)



Not Secure
rosetta.oats.inaf.it:7000/vnc.html?autoconnect=true&resize=remote
Terminal
File Edit View Terminal Tabs Help
Terminal

```
Singularity> 
```

Rosetta quickstart & demo (for users)



Not Secure
rosetta.oats.inaf.it:7000/vnc.html?autoconnect=true&resize=remote
Terminal - IPython:
File Edit View Terminal Tabs Help
IPython: datasets/MKN509
Viewer Display Panel (BN)
Data Display Panel Tools View Help
Display
Animators
Channels
Images
Cursors
Regions
MKN509.central.mfs.image.fits–raster
–331.789 km/s
ICRS Declination
ICRS Right Ascension
50"
43'00"
10"
20"
30"
40"
50"
–10°44'00"
20ʰ44ᵐ12ˢ
11ˢ
10ˢ
09ˢ
08ˢ
close
☑ leave
Terminal - IPython: datasets/MKN509
Log Messages (:/data_sarusso/datasets/MKN509/casa
Viewer Display Panel (BN)
Data Manager -- Viewer

```
perl: warning: Setting locale failed.
perl: warning: Please check that your lo
        LANGUAGE = (unset),
        LC_ALL = (unset),
        LC_NUMERIC = "en_US.UTF-8",
        LANG = "C"
    are supported and installed on your
perl: warning: Falling back to the stand
perl: warning: Setting locale failed.
perl: warning: Please check that your lo
        LANGUAGE = (unset),
        LC_ALL = (unset),
        LC_NUMERIC = "en_US.UTF-8",
        LANG = "C"
    are supported and installed on your
perl: warning: Falling back to the stand
--> CrashReporter initialized.
Enter doc('start') for help getting star
Using matplotlib backend: TkAgg

CASA <1>: viewer()


CASA <2>: 
```

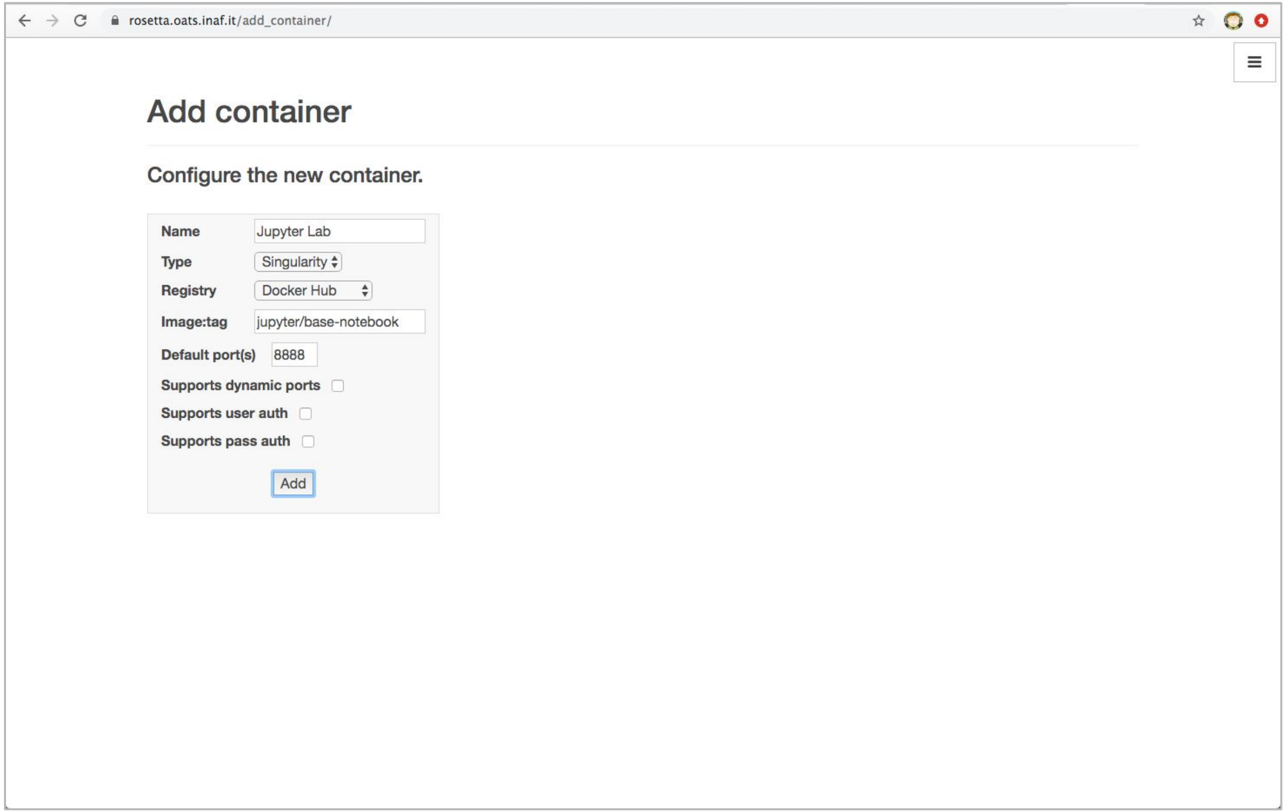
```
MKN509.central.hogbom.image.fits    FITS Image
MKN509.central.mfs.image.fits       FITS Image
MKN509.csub.briggs-05.image         Image
MKN509.csub.briggs-05.image.fits    FITS Image
MKN509.csub.briggs-05.mask          Image
MKN509.csub.briggs-05.model         Image
MKN509.csub.briggs-05.pb            Image
MKN509.csub.briggs-05.psf           Image
MKN509.csub.briggs-05.residual      Image
MKN509.csub.briggs-05.sumwt         Image
```

□ slice

☑ MKN509.central.mfs.image.fits-raster

```
masked                   Pixel: 76 67 0 0
20:44:12.077  -10.43.58.914  -331.789 km/s   (lsrk/radio velocity) I
```

Rosetta quickstart & demo (for users)

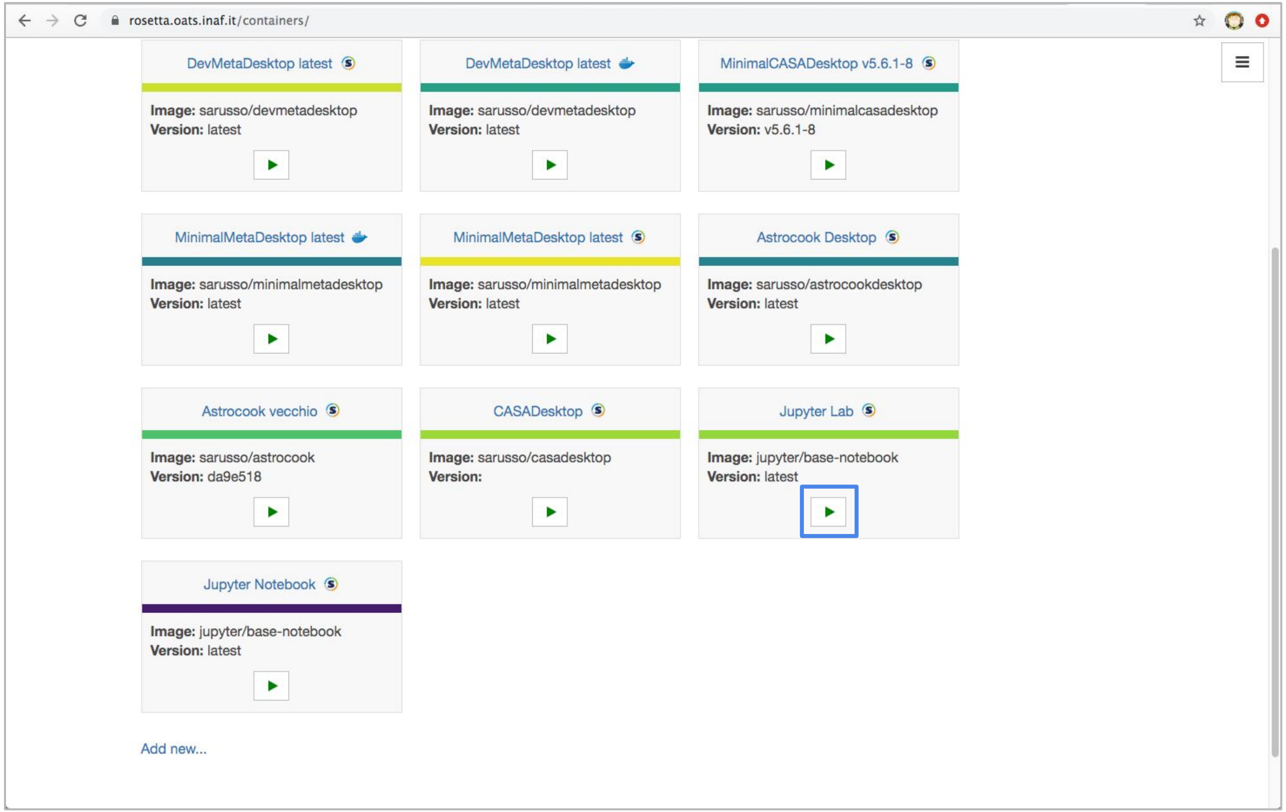


Add container

Configure the new container.

Name	Jupyter Lab
Type	Singularity
Registry	Docker Hub
Image:tag	jupyter/base-notebook
Default port(s)	8888
Supports dynamic ports	□
Supports user auth	□
Supports pass auth	□

Rosetta quickstart & demo (for users)



DevMetaDesktop latest

Image: sarusso/devmetadesktop
Version: latest

DevMetaDesktop latest

Image: sarusso/devmetadesktop
Version: latest

MinimalCASADesktop v5.6.1-8

Image: sarusso/minimalcasadesktop
Version: v5.6.1-8

MinimalMetaDesktop latest

Image: sarusso/minimalmetadesktop
Version: latest

MinimalMetaDesktop latest

Image: sarusso/minimalmetadesktop
Version: latest

Astrocook Desktop

Image: sarusso/astrocookdesktop
Version: latest

Astrocook vecchio

Image: sarusso/astrocook
Version: da9e518

CASADesktop

Image: sarusso/casadesktop
Version:

Jupyter Lab

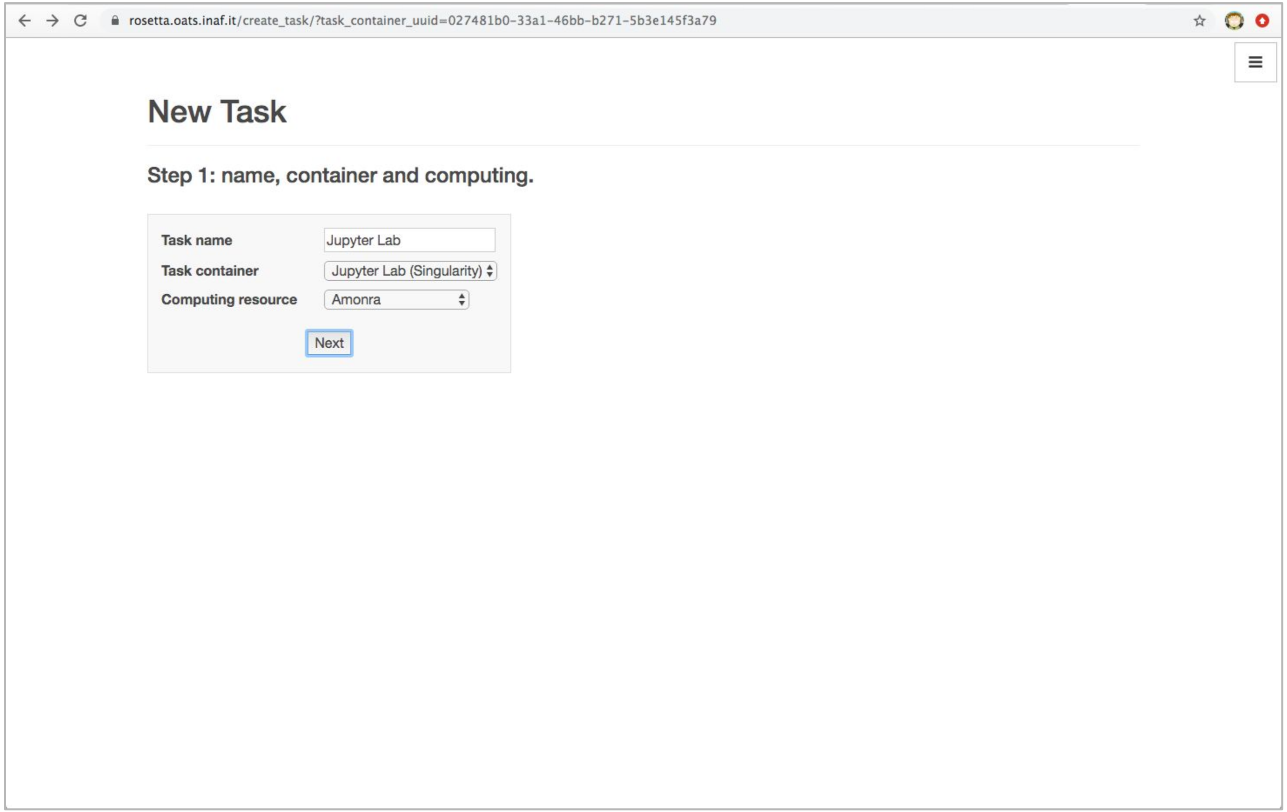
Image: jupyter/base-notebook
Version: latest

Jupyter Notebook

Image: jupyter/base-notebook
Version: latest

Add new...

Rosetta quickstart & demo (for users)



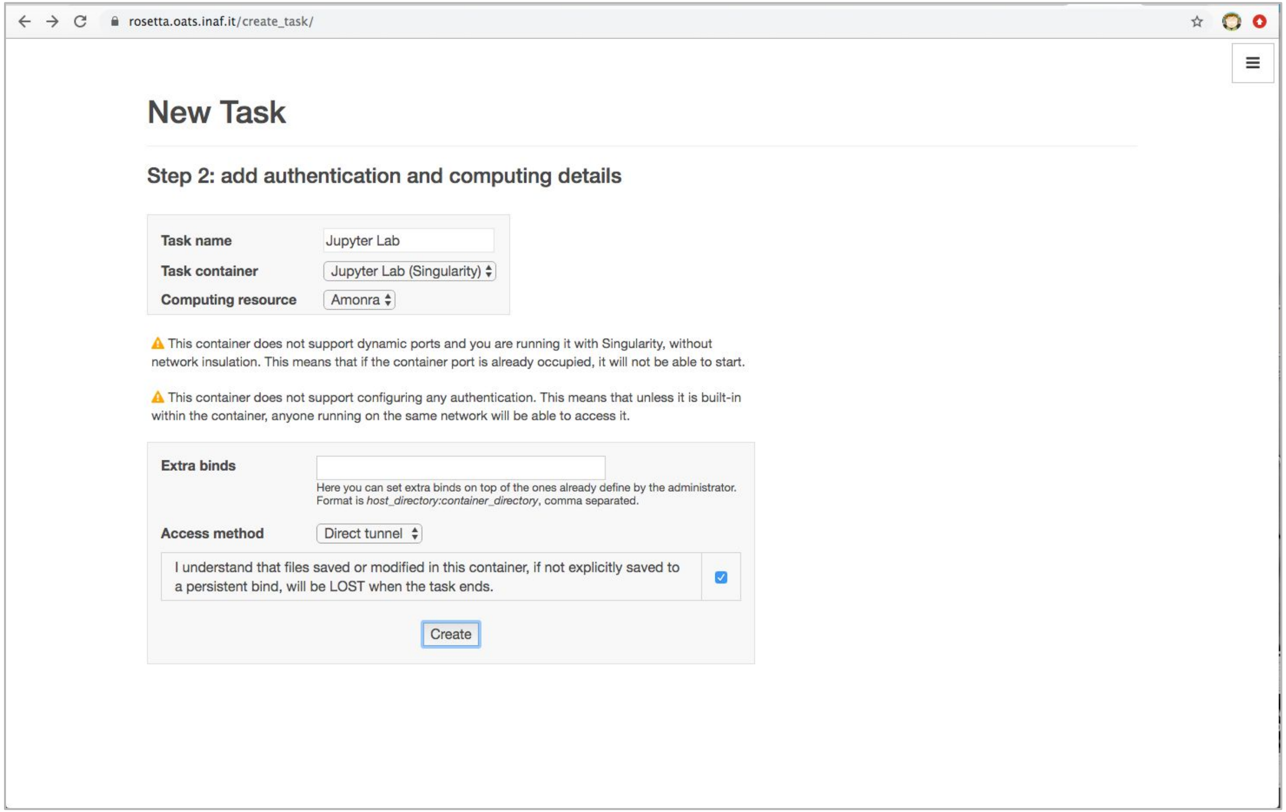
rosetta.oats.inaf.it/create_task/?task_container_uuid=027481b0-33a1-46bb-b271-5b3e145f3a79

New Task

Step 1: name, container and computing.

Task name	Jupyter Lab
Task container	Jupyter Lab (Singularity)
Computing resource	Amonra

Rosetta quickstart & demo (for users)



New Task

Step 2: add authentication and computing details

Task name	Jupyter Lab
Task container	Jupyter Lab (Singularity)
Computing resource	Amonra

⚠ This container does not support dynamic ports and you are running it with Singularity, without network insulation. This means that if the container port is already occupied, it will not be able to start.

⚠ This container does not support configuring any authentication. This means that unless it is built-in within the container, anyone running on the same network will be able to access it.

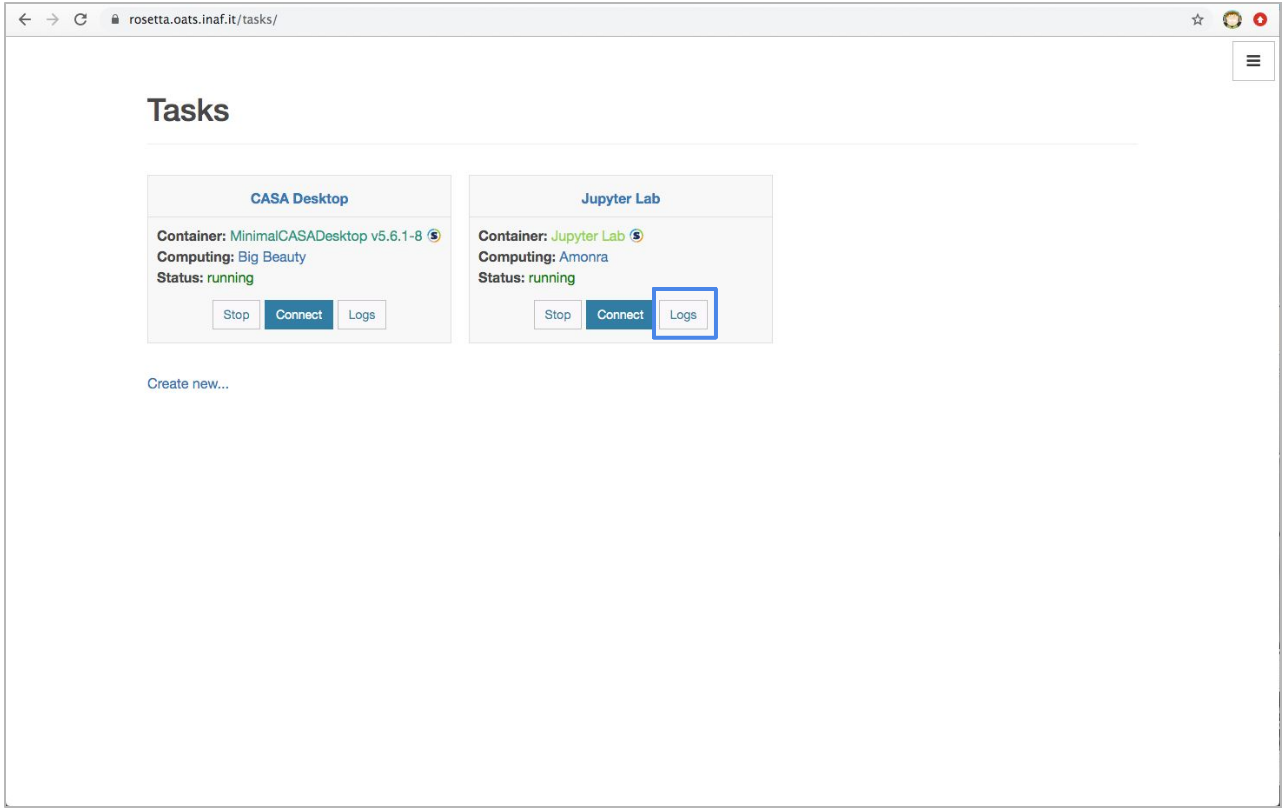
Extra binds

Here you can set extra binds on top of the ones already define by the administrator. Format is *host_directory:container_directory*, comma separated.

Access method Direct tunnel

I understand that files saved or modified in this container, if not explicitly saved to a persistent bind, will be LOST when the task ends. ☑

Rosetta quickstart & demo (for users)



rosetta.oats.inaf.it/tasks/

Tasks

CASA Desktop

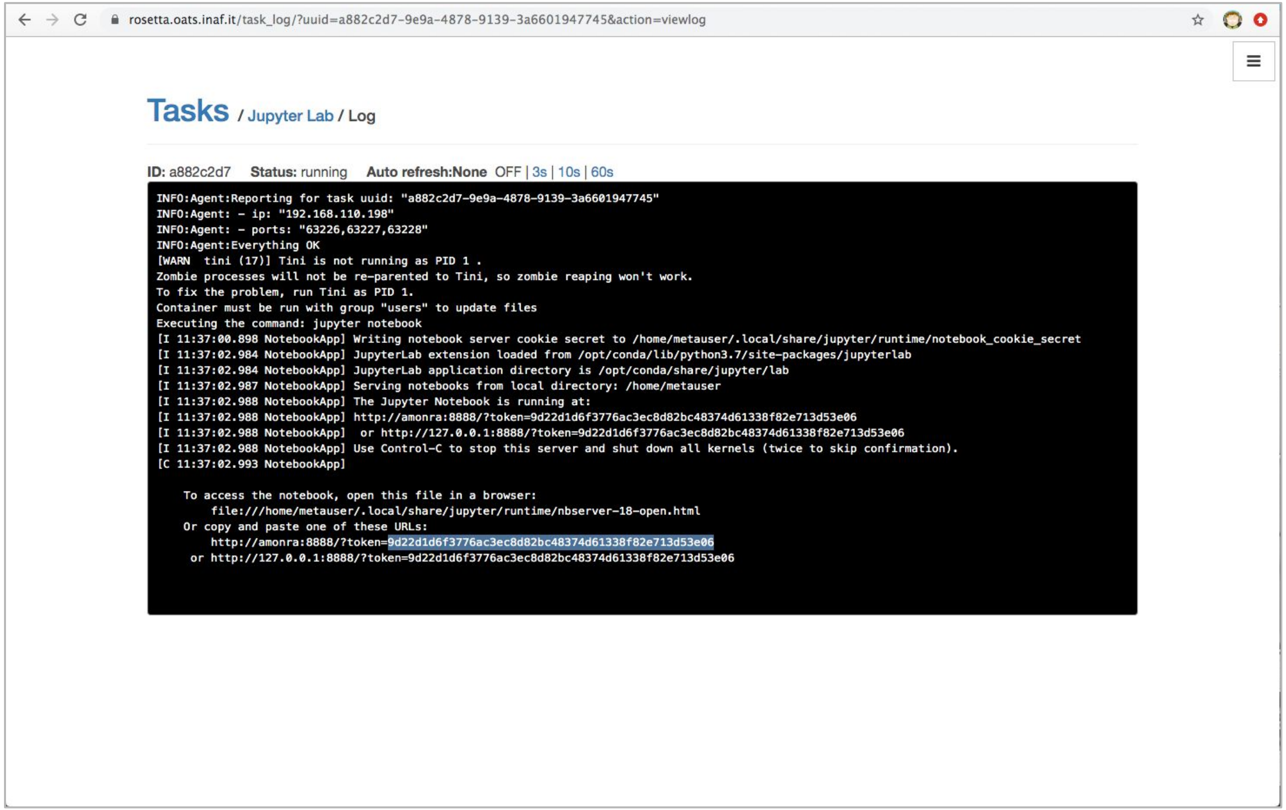
Container: MinimalCASADesktop v5.6.1-8
Computing: Big Beauty
Status: running

Jupyter Lab

Container: Jupyter Lab
Computing: Amonra
Status: running

Create new...

Rosetta quickstart & demo (for users)



rosetta.oats.inaf.it/task_log/?uuid=a882c2d7-9e9a-4878-9139-3a6601947745&action=viewlog

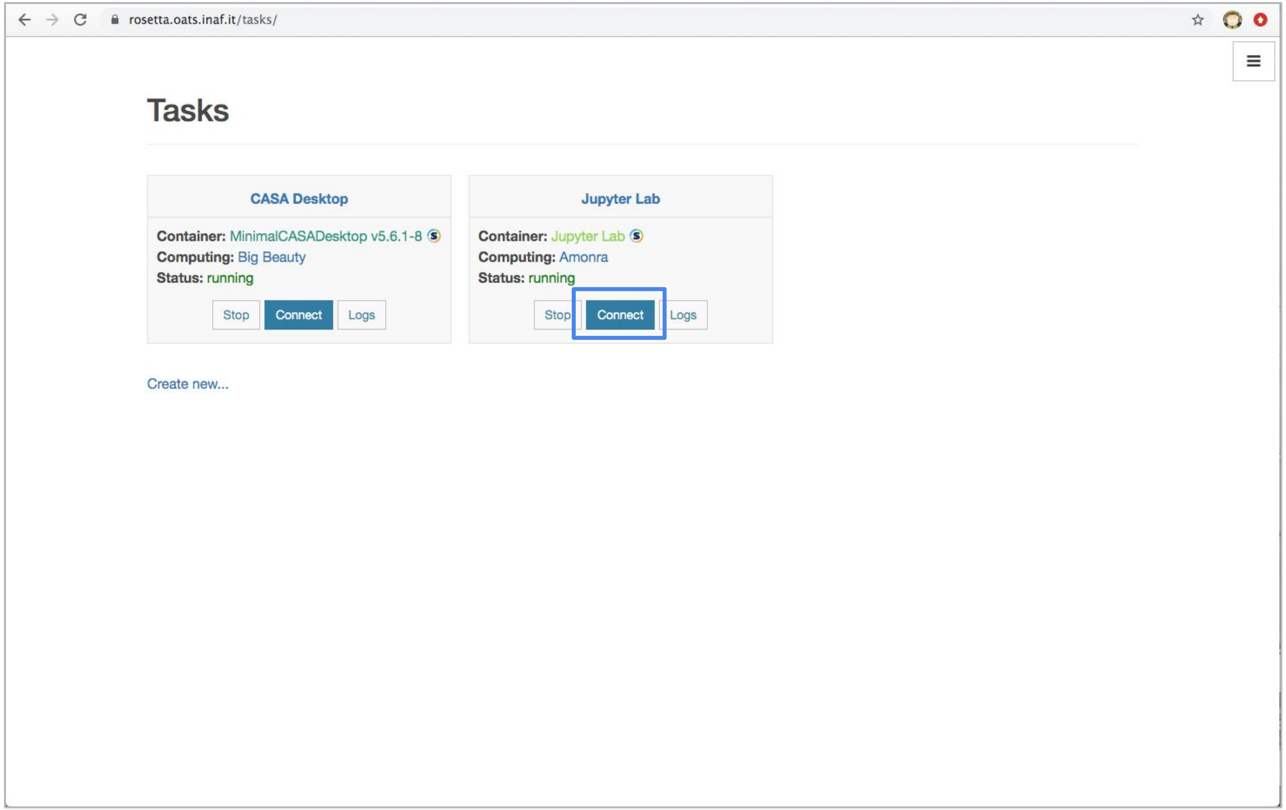
Tasks / Jupyter Lab / Log

ID: a882c2d7 **Status:** running **Auto refresh:None** OFF | 3s | 10s | 60s

```
INFO:Agent:Reporting for task uuid: "a882c2d7-9e9a-4878-9139-3a6601947745"
INFO:Agent: - ip: "192.168.110.198"
INFO:Agent: - ports: "63226,63227,63228"
INFO:Agent:Everything OK
[WARN  tini (17)] Tini is not running as PID 1 .
Zombie processes will not be re-parented to Tini, so zombie reaping won't work.
To fix the problem, run Tini as PID 1.
Container must be run with group "users" to update files
Executing the command: jupyter notebook
[I 11:37:00.898 NotebookApp] Writing notebook server cookie secret to /home/metauser/.local/share/jupyter/runtime/notebook_cookie_secret
[I 11:37:02.984 NotebookApp] JupyterLab extension loaded from /opt/conda/lib/python3.7/site-packages/jupyterlab
[I 11:37:02.984 NotebookApp] JupyterLab application directory is /opt/conda/share/jupyter/lab
[I 11:37:02.987 NotebookApp] Serving notebooks from local directory: /home/metauser
[I 11:37:02.988 NotebookApp] The Jupyter Notebook is running at:
[I 11:37:02.988 NotebookApp] http://amonra:8888/?token=9d22d1d6f3776ac3ec8d82bc48374d61338f82e713d53e06
[I 11:37:02.988 NotebookApp]  or http://127.0.0.1:8888/?token=9d22d1d6f3776ac3ec8d82bc48374d61338f82e713d53e06
[I 11:37:02.988 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 11:37:02.993 NotebookApp]

    To access the notebook, open this file in a browser:
        file:///home/metauser/.local/share/jupyter/runtime/nbserver-18-open.html
    Or copy and paste one of these URLs:
        http://amonra:8888/?token=9d22d1d6f3776ac3ec8d82bc48374d61338f82e713d53e06
     or http://127.0.0.1:8888/?token=9d22d1d6f3776ac3ec8d82bc48374d61338f82e713d53e06
```

Rosetta quickstart & demo (for users)



rosetta.oats.inaf.it/tasks/

Tasks

CASA Desktop

Container: MinimalCASADesktop v5.6.1-8
Computing: Big Beauty
Status: running

Stop Connect Logs

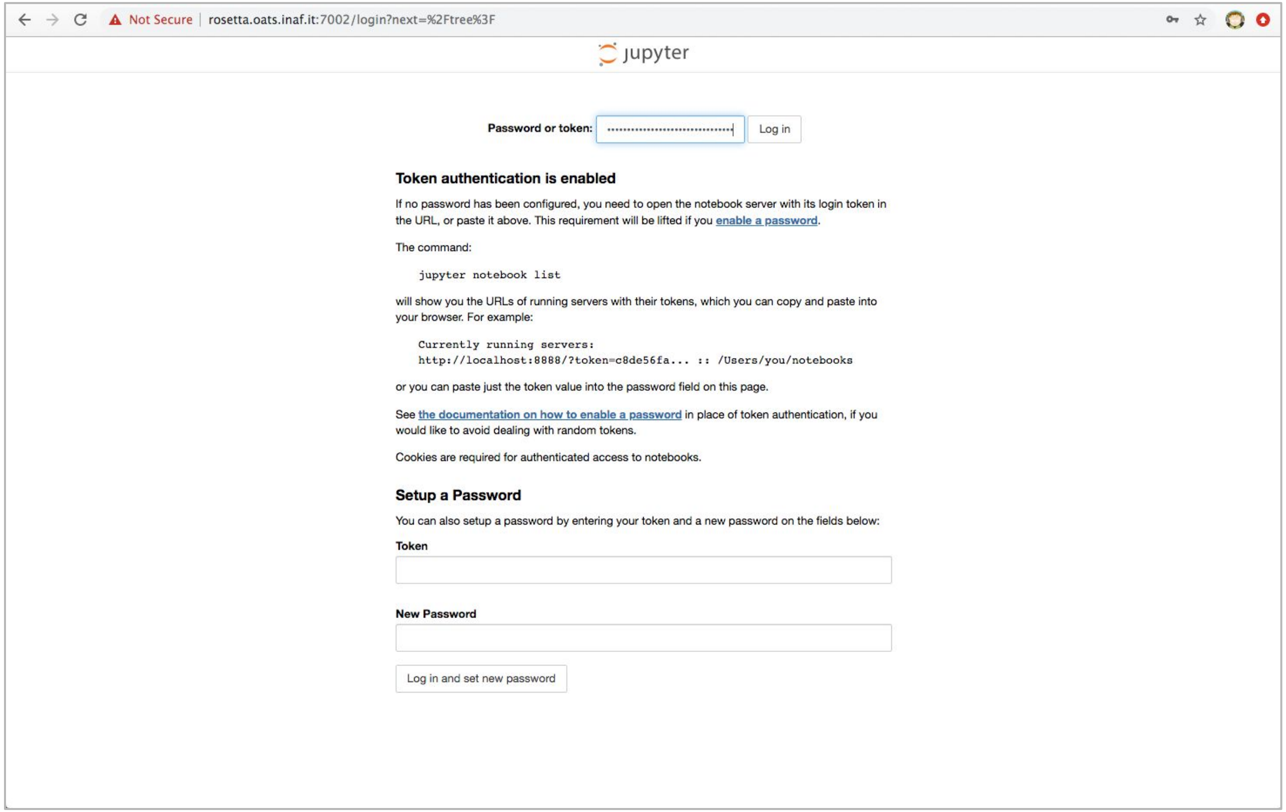
Jupyter Lab

Container: Jupyter Lab
Computing: Amonra
Status: running

Stop Connect Logs

Create new...

Rosetta quickstart & demo (for users)



Password or token: •••••••••••••••••••••••••••••••••• Log in

Token authentication is enabled

If no password has been configured, you need to open the notebook server with its login token in the URL, or paste it above. This requirement will be lifted if you enable a password.

The command:

```
jupyter notebook list
```

will show you the URLs of running servers with their tokens, which you can copy and paste into your browser. For example:

```
Currently running servers:
http://localhost:8888/?token=c8de56fa... :: /Users/you/notebooks
```

or you can paste just the token value into the password field on this page.

See the documentation on how to enable a password in place of token authentication, if you would like to avoid dealing with random tokens.

Cookies are required for authenticated access to notebooks.

Setup a Password

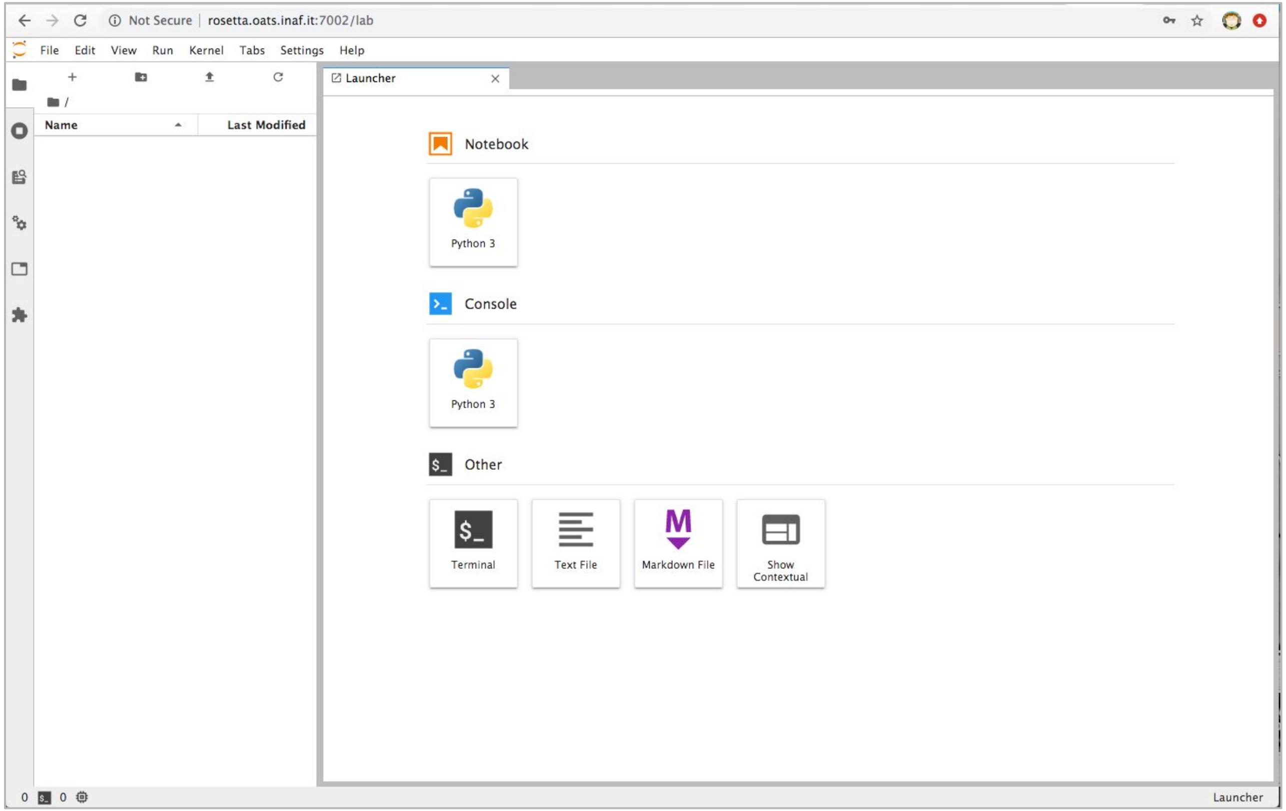
You can also setup a password by entering your token and a new password on the fields below:

Token

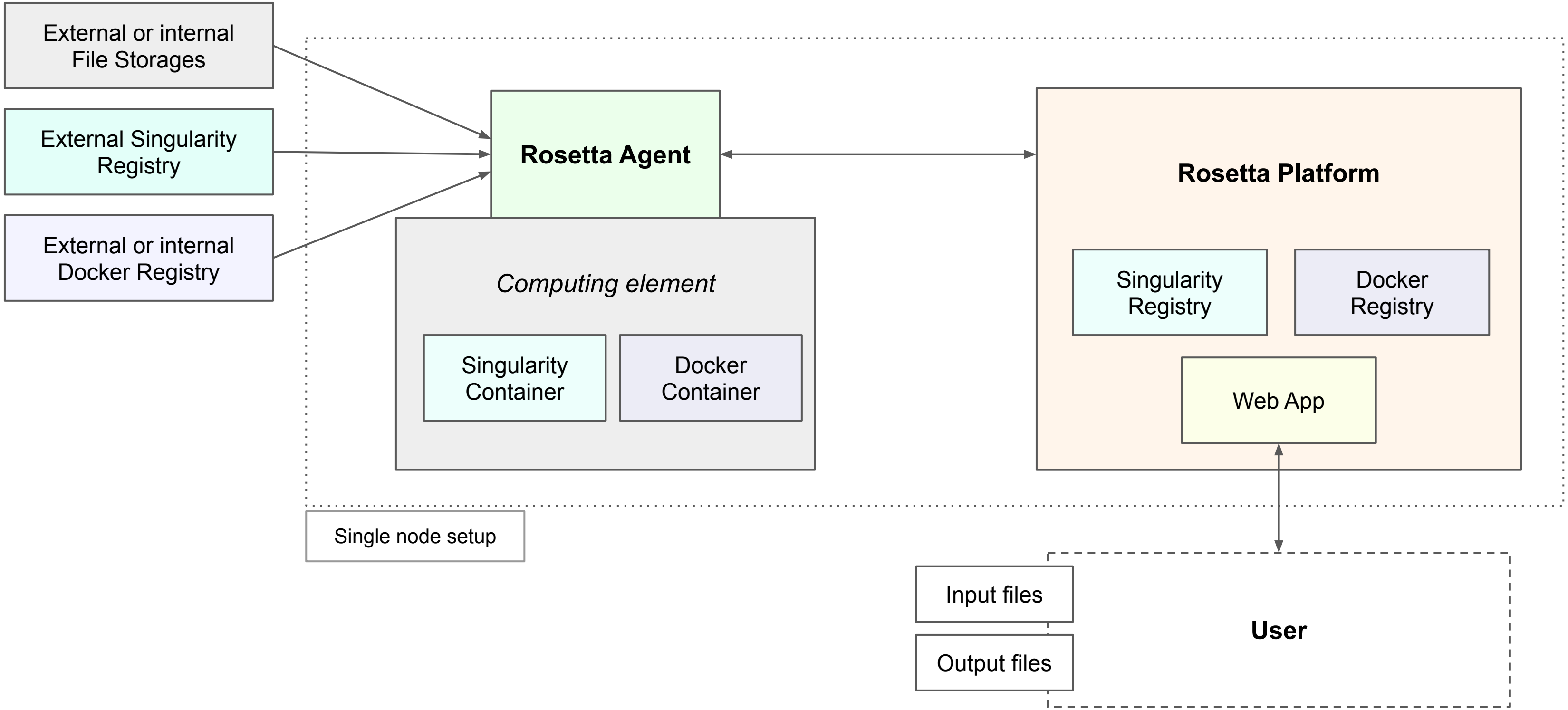
New Password

Log in and set new password

Rosetta quickstart & demo (for users)



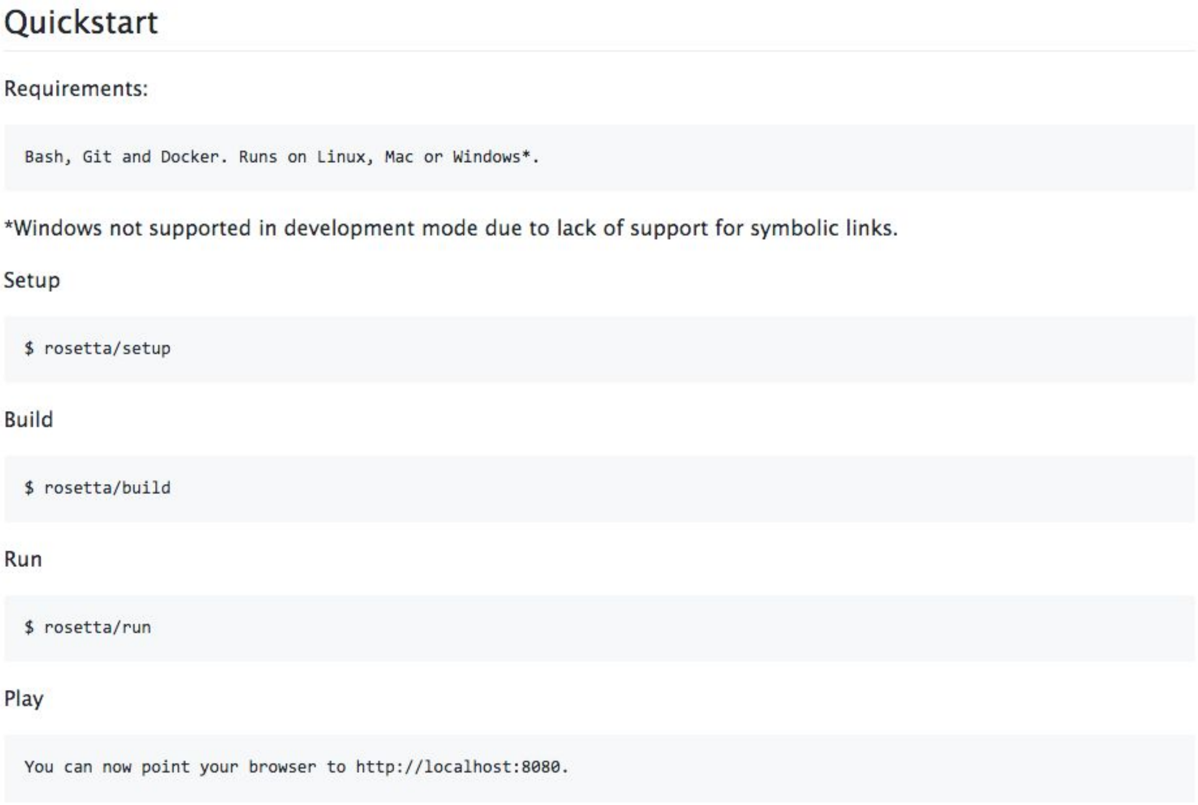
Rosetta Architecture



Rosetta technology stack

1. Docker + docker compose for orchestrating Rosetta itself
2. Python + Django for the orchestration
3. HTML for the Webapp
4. REST APIs (in development)
5. Postgres (or SQLite) database

Rosetta quickstart (for devs)



Quickstart

Requirements:

```
Bash, Git and Docker. Runs on Linux, Mac or Windows*.
```

*Windows not supported in development mode due to lack of support for symbolic links.

Setup

```
$ rosetta/setup
```

Build

```
$ rosetta/build
```

Run

```
$ rosetta/run
```

Play

```
You can now point your browser to http://localhost:8080.
```

Rosetta status

- Deployed on rosetta.inaf.oats.it, invite-based only for power-users beta tester
- A few user from other institutes using it autonomously on their own laptops for its orchestration capabilities

  → (i.e. to easily access remote desktops when locked out from offices in the pandemic.)
- Supports Singularity containers with preliminary support for Docker.
- Ships “batteries included”, with a few containers preconfigured and a test Slurm cluster instance up & running

That’s it :)

Questions?

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Rosetta repository: https://github.com/sarusso/Rosetta