



Open Science on Cloud using Jupyter Notebooks

Cloud workflows with NaaVRE

Concepts, tutorial and exercises

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(LifeWatch ERIC VLIC / MNS, University of Amsterdam)

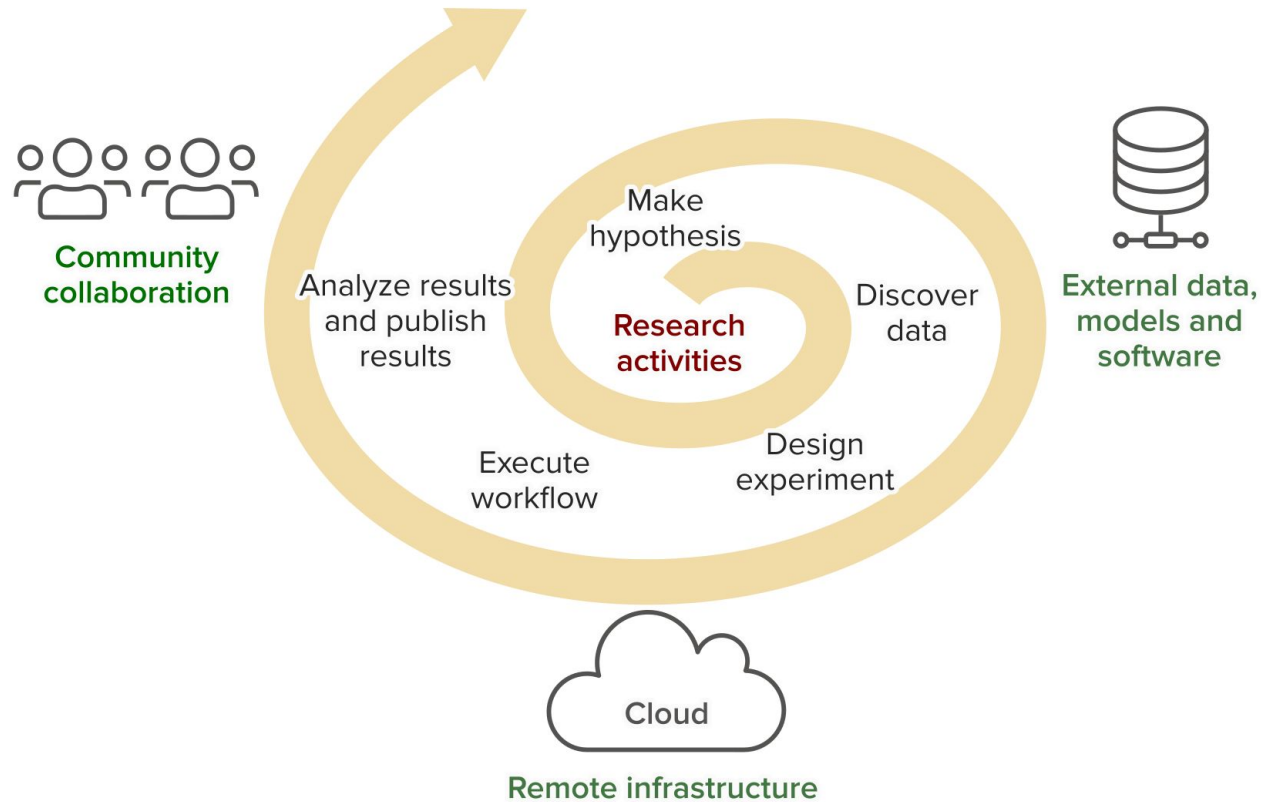
25/06/2025



IR0000032 – ITINERIS, Italian Integrated Environmental Research Infrastructures System
(D.D. n. 130/2022 - CUP B53C22002150006) Funded by EU - Next Generation EU PNRR-
Mission 4 "Education and Research" - Component 2: "From research to business" - Investment
3.1: "Fund for the realisation of an integrated system of research and innovation infrastructures"



Data-centric research lifecycle



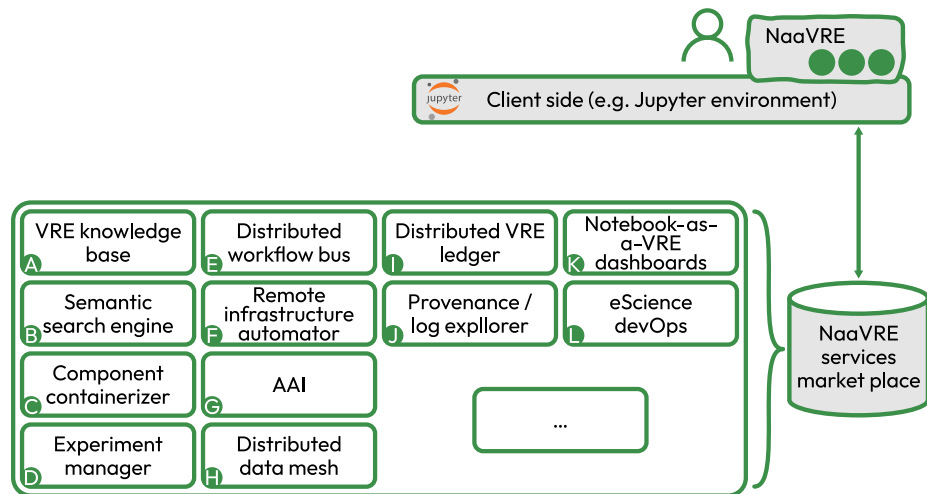
"Virtual Research Environments (VREs) provide user-centric support for discovering and selecting data and software services from different sources and composing and executing application workflows, ..." (Jeffery et al., 2020)

How to support data-centric experiments

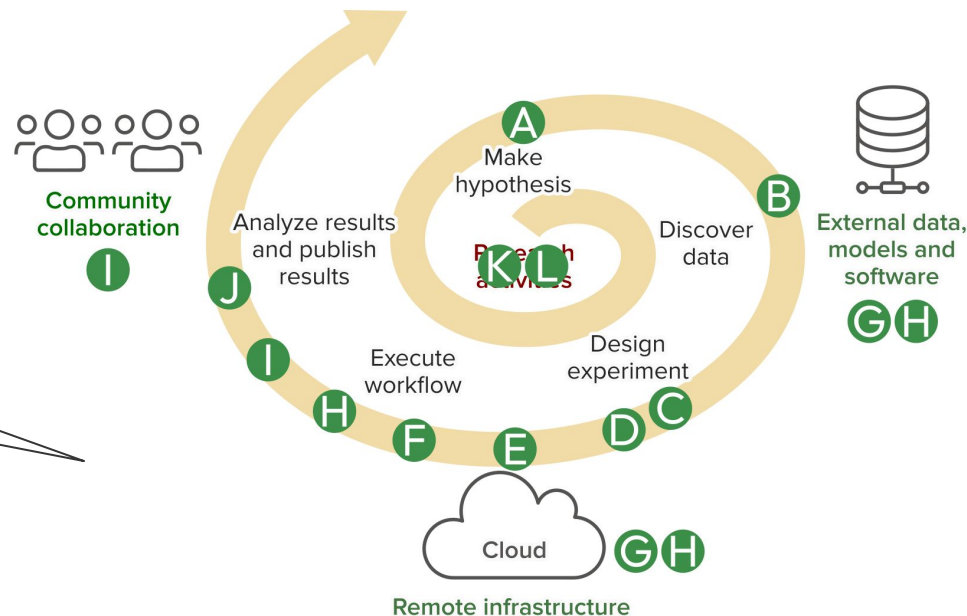
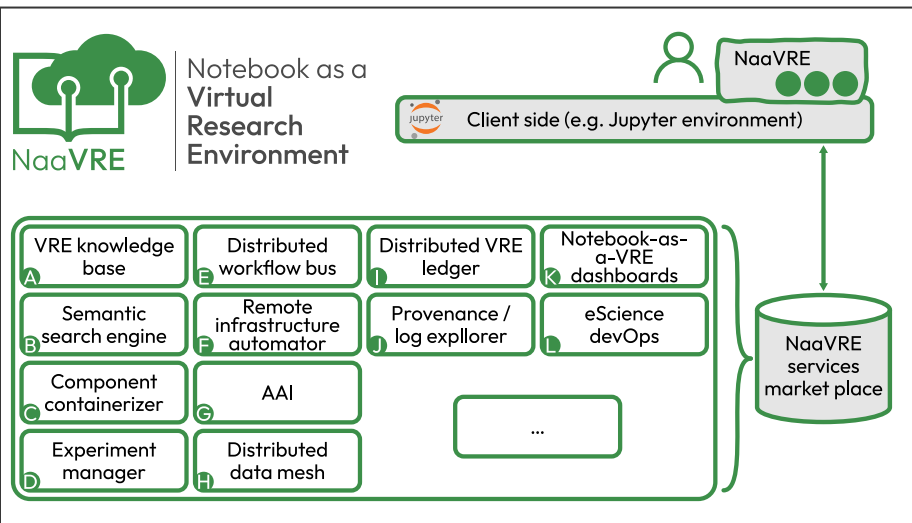
- **Computational notebooks**
 - Widely used by researchers
 - Documentation and visualization alongside code
 - Interactive code execution
 - → **developing and tweaking models**
- **Virtual research environment**
 - Collaboration
 - FAIR data, models and services
 - Remote infrastructure
 - Scaling up models (e.g. porting prototype to large-scale cloud environment)
 - → **sharing mature models & more**
- **Combined, they are NaaVRE**



Notebook as a
**Virtual
Research
Environment**

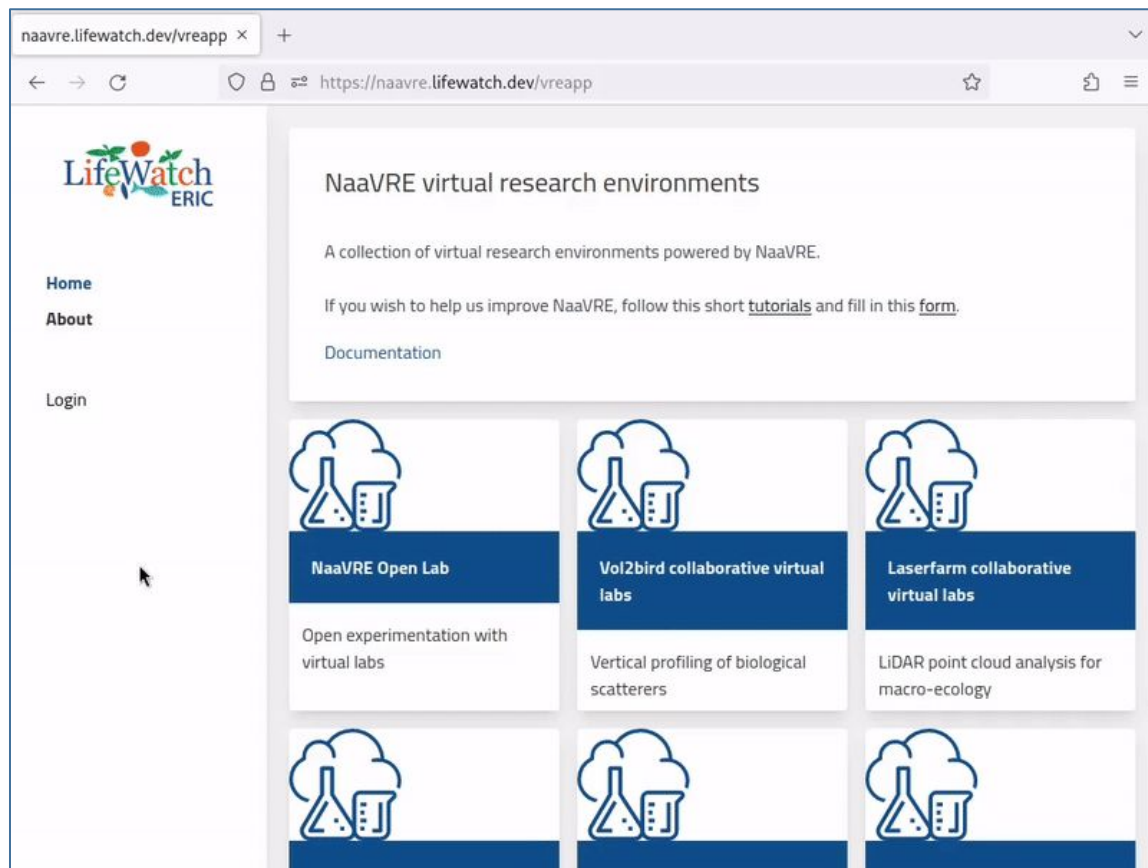
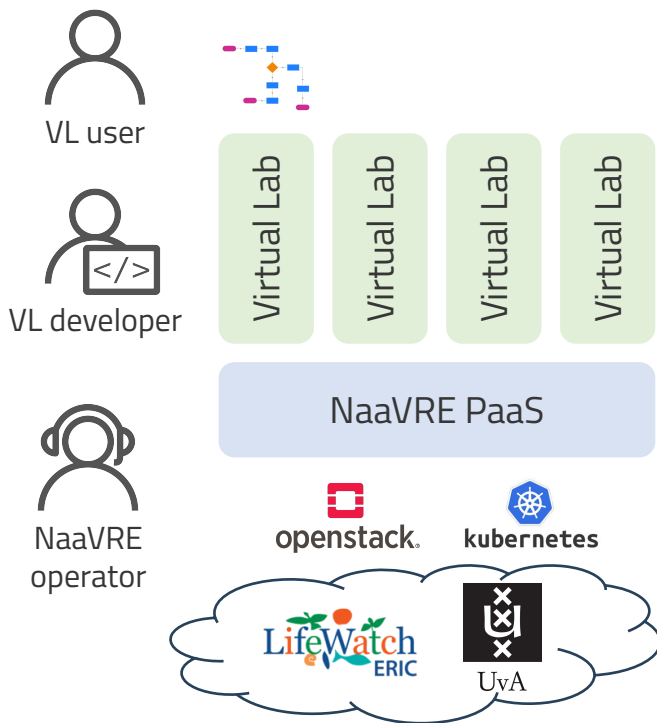


Research activities and Jupyter extensions



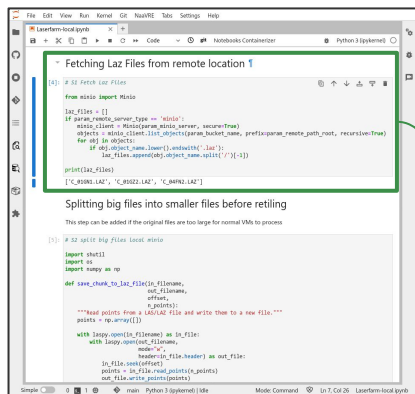
Zhao, Z., Koulouzis, S., Bianchi, R., Farshidi, S., Shi, Z., Xin, R., Wang, Y., Li, N., Shi, Y., Timmermans, J., Kissling, W.D.: Notebook-as-a-VRE (NaaVRE): From private notebooks to a collaborative cloud virtual research environment. Softw Pract Exp. spe.3098 (2022). <https://doi.org/10.1002/spe.3098>.

Notebook-as-a-VRE and Virtual Labs



From notebooks to cloud workflows

1. PROTOTYPE MODEL IN NOTEBOOK



```
from lazrs import LazFile

def fetch_laz_files(remote_location):
    """Fetch Laz files from remote location"""
    # Fetch Laz files from remote location
    laz_files = []
    if param_remote_server_type == "minio":
        minio_client = MinioClient(param_minio_server, secure=True)
        objects = minio_client.list_objects(param_bucket_name, prefix=param_remote_path_root, recursive=True)
        for obj in objects:
            if obj.object_name.lower().endswith(".laz"):
                laz_files.append(obj.object_name.split("/")[-1])
    print(laz_files)

    ["C:\RINGS_LAZ", "C:\RINGS_LAZ", "C:\RINGS_LAZ"]

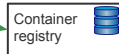
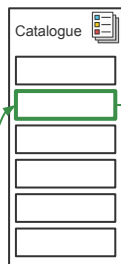
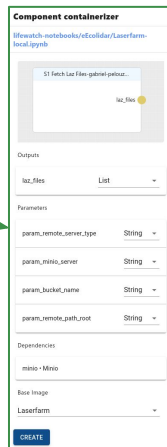
def split_big_files_local_minio():
    """Split big files into smaller files before retiling"""
    This step can be added if the original files are too large for normal VMs to process

    # Split big files local minio
    import shutil
    import os
    import sys as sys

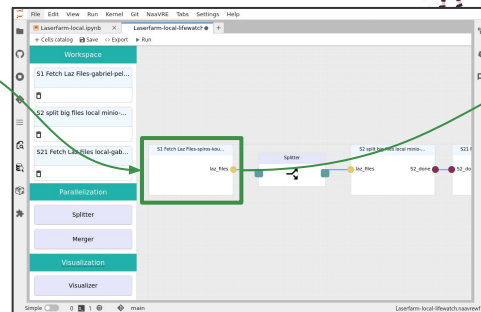
    def save_chunk_to_laz_file(in_filename, out_filename, offset):
        """Save chunk to laz file"""
        points = []
        with open(in_filename) as in_file:
            header = in_file.readline()
            points = in_file.readlines()
            out_file = open(out_filename, "w")
            out_file.write(header)
            out_file.write(points)

    # Split big files local minio
```

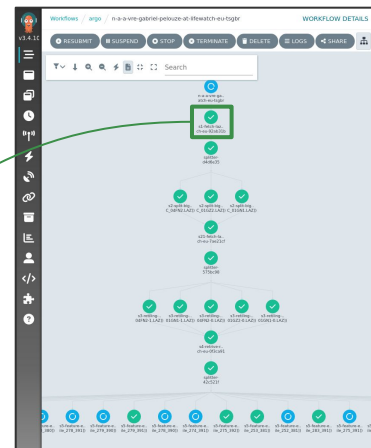
2. CONTAINERIZE CELLS



3. COMPOSE A WORKFLOW



4. RUN IT IN THE CLOUD

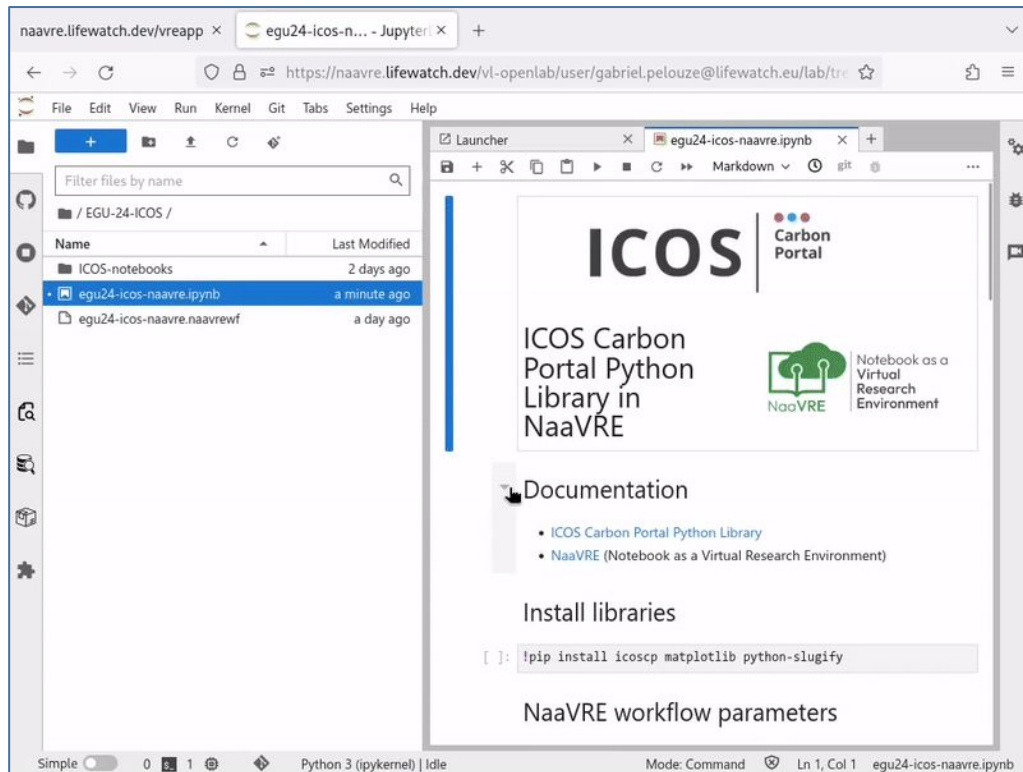


From notebooks to cloud workflows

1. PROTOTYPE MODEL IN NOTEBOOK

2. CONTAINERIZE CELLS

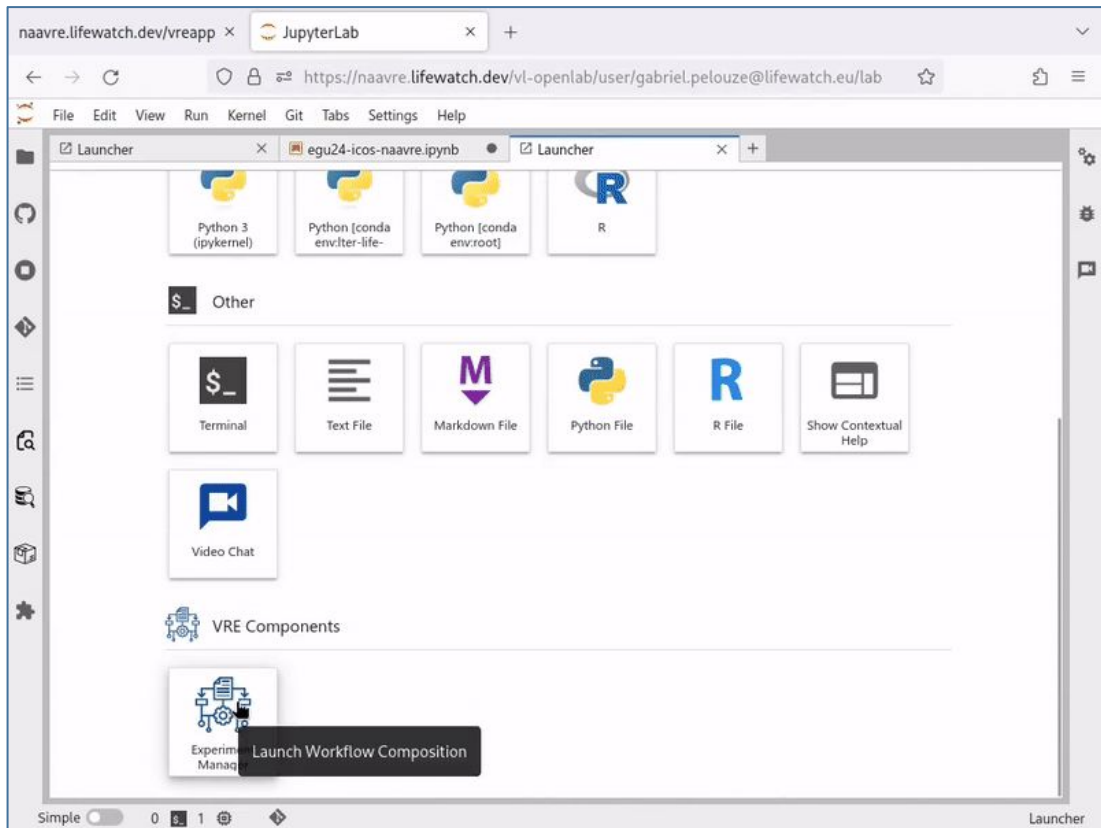
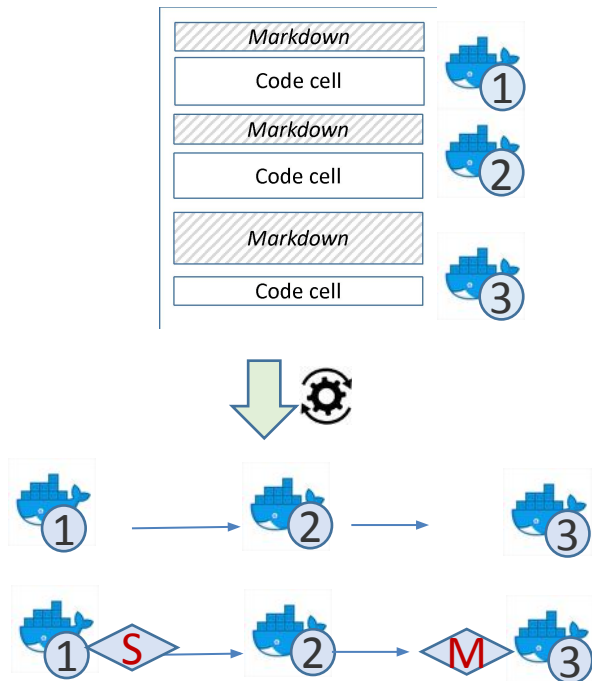
Encapsulate **user-selected cells** as standardized services and **containerize** them as **reusable components**.



From notebooks to cloud workflows

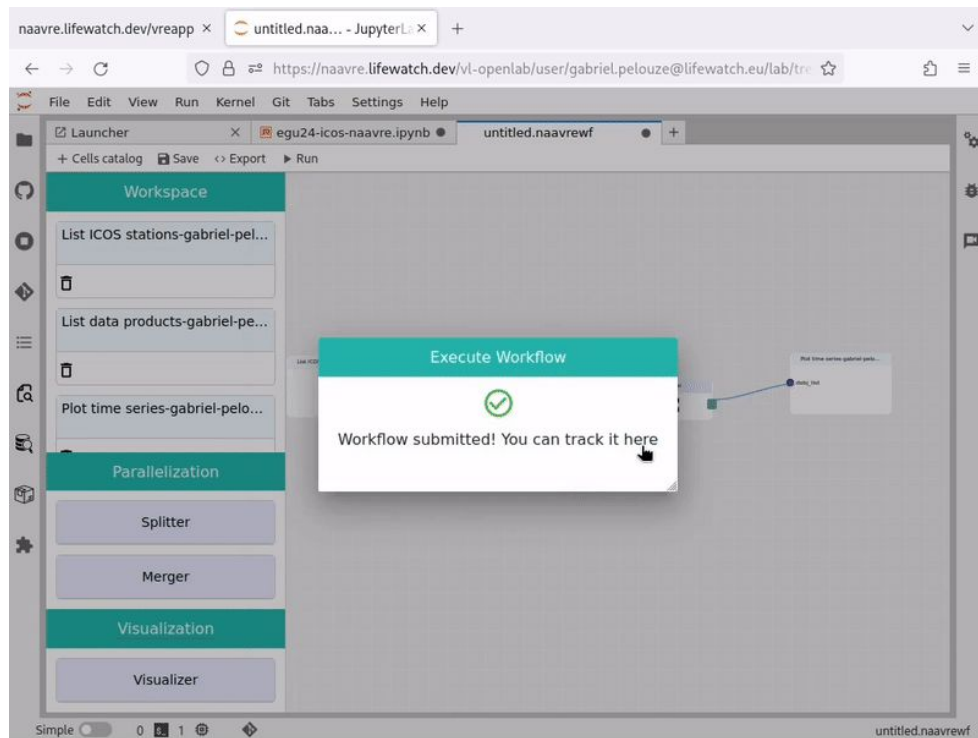
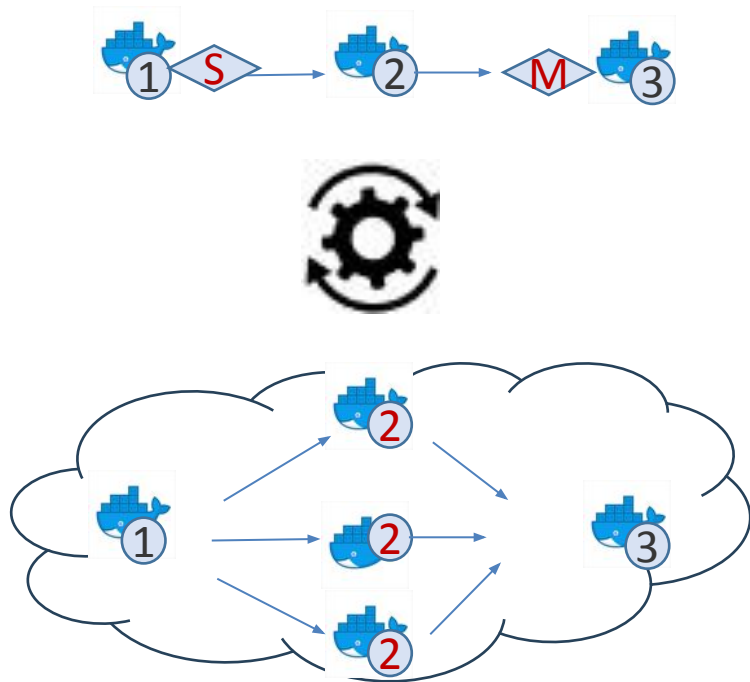
3. COMPOSE A WORKFLOW: Customize data flow and input

An experiment is a workflow of services, with customized input data and infrastructure

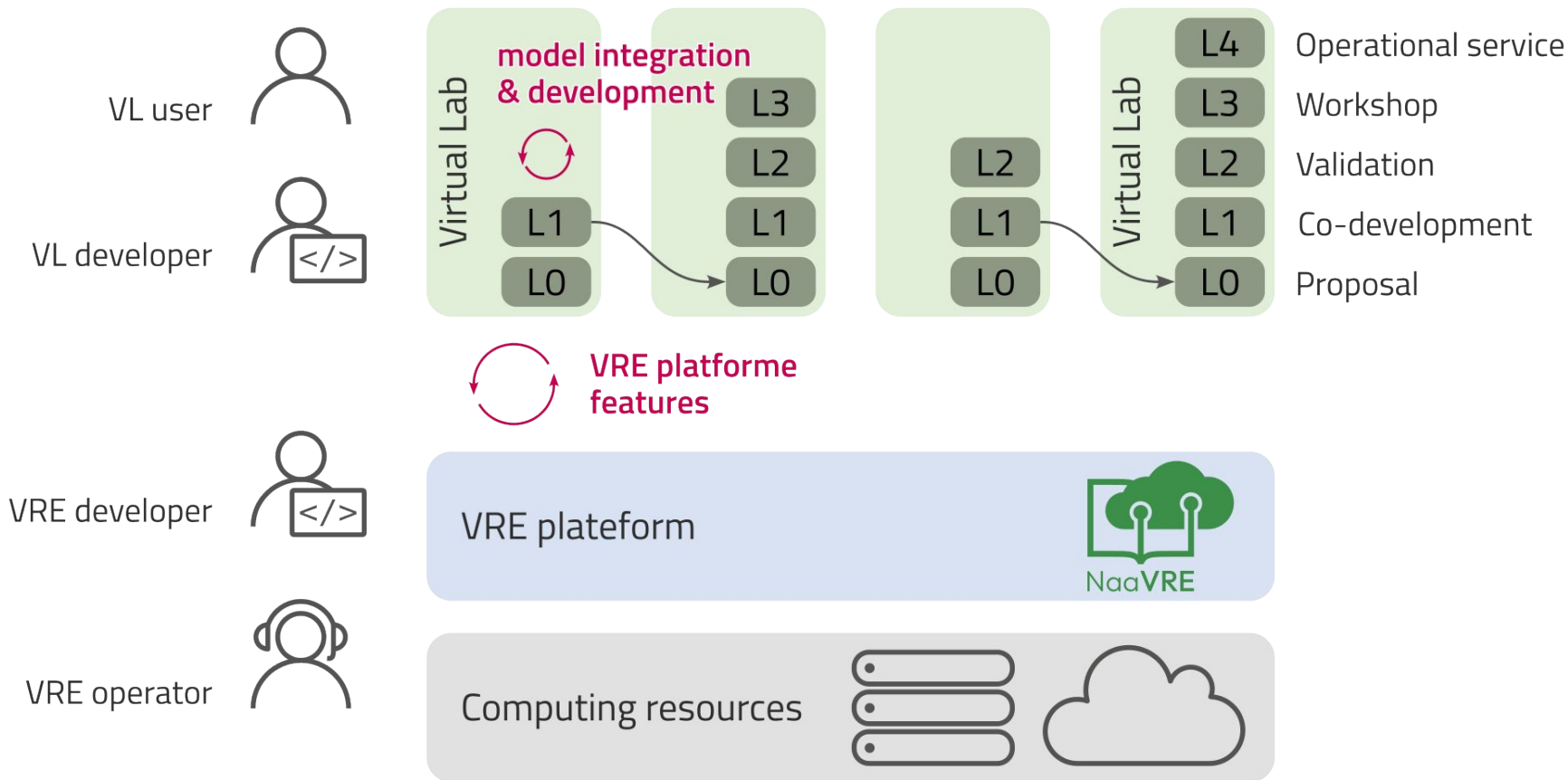


From notebooks to cloud workflows

4. RUN THE WORKFLOW: Automate the workflow components deployment and execution



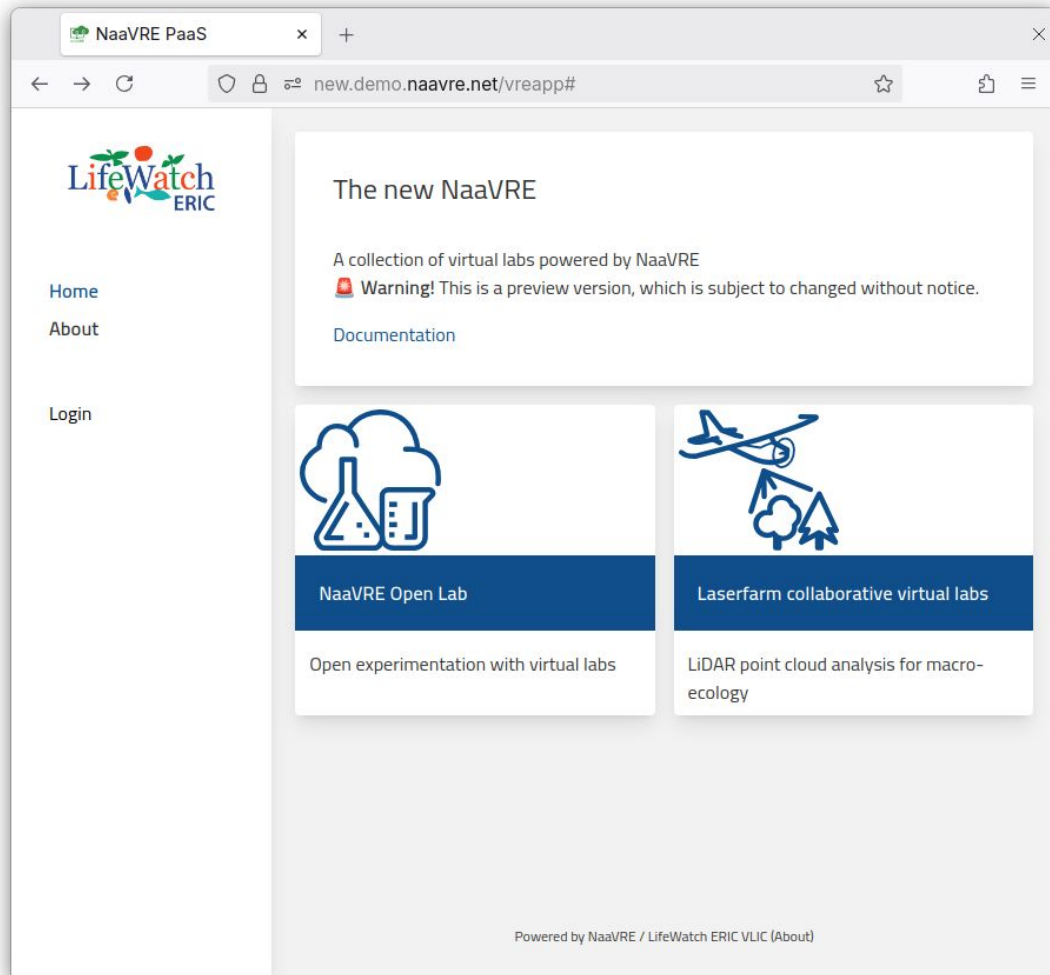
VRE and Virtual Lab co-development framework




Hands-on NaaVRE

Starting point

Get started at
<https://new.demo.naavre.net>




Sign in



Home

About


Login 

NaaVRE virtual research environment

A collection of virtual research environments powered by LifeWatch ERIC


If you wish to help us improve NaaVRE follow this [tutorial](#) and fill in this [form](#).

[Documentation](#)




NaaVRE Open Lab

Open experimentation with virtual labs




Vol2bird collaborative virtual labs

Vertical profile scatterers




Laserfarm collaborative virtual labs

LiDAR point cloud analysis for



Veluwe project

Veluwe Digital LTER-LIFE



Sign in to your account

Email


Password


☐ Remember me [Forgot Password?](#)

[Sign In](#)


Or sign in with

LifeWatch ERIC

 Google

Federation w 

New user? [Register](#)

 Sign in with Google

Sign in

to continue to lifewatch.eu

Email or phone

[Forgot email?](#)

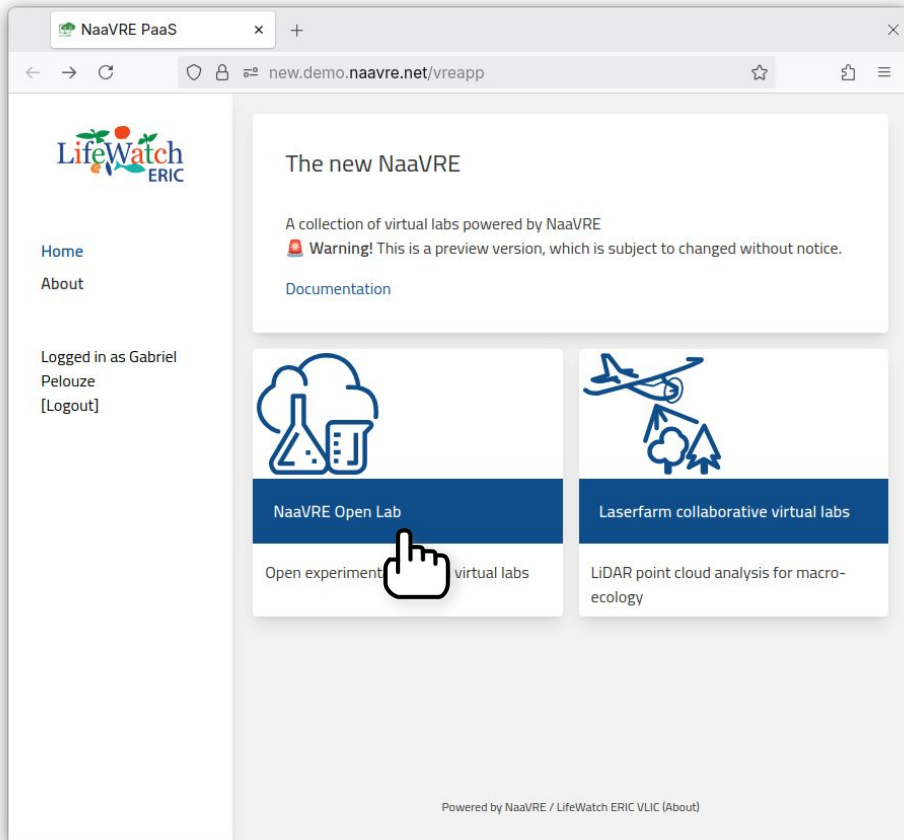
To continue, Google will share your name, email address, language preference, and profile picture with lifewatch.eu. Before using this app, you can review lifewatch.eu's [privacy policy](#) and [terms of service](#).

[Create account](#) [Next](#)

English (United States) ▼

[Help](#) [Privacy](#) [Terms](#)

Pick your collaborative virtual labs



The screenshot shows the NaaVRE PaaS homepage. The browser address bar displays 'new.demo.naavre.net/vreapp'. The page features the LifeWatch ERIC logo and a navigation menu with 'Home' and 'About'. A sidebar on the left indicates the user is logged in as 'Gabriel Pelouze' and provides a '[Logout]' link. The main content area is titled 'The new NaaVRE' and includes a warning: 'Warning! This is a preview version, which is subject to change without notice.' Below this, there are two prominent buttons: 'NaaVRE Open Lab' and 'Laserfarm collaborative virtual labs'. A hand cursor is positioned over the 'NaaVRE Open Lab' button. The footer states 'Powered by NaaVRE / LifeWatch ERIC VLIC (About)'.

NaaVRE PaaS

new.demo.naavre.net/vreapp

LifeWatch ERIC

Home

About

Logged in as Gabriel Pelouze [Logout]

The new NaaVRE

A collection of virtual labs powered by NaaVRE

Warning! This is a preview version, which is subject to change without notice.

Documentation

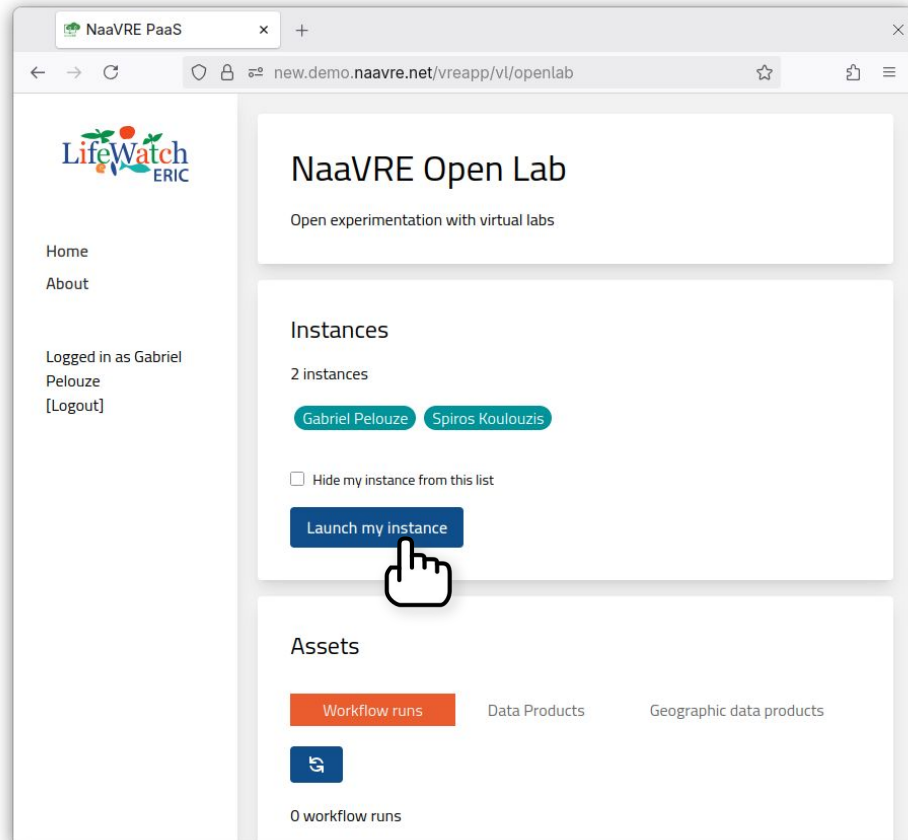
NaaVRE Open Lab

Open experimentation with virtual labs

Laserfarm collaborative virtual labs

LiDAR point cloud analysis for macro-ecology

Powered by NaaVRE / LifeWatch ERIC VLIC (About)



The screenshot shows the NaaVRE Open Lab interface. The browser address bar displays 'new.demo.naavre.net/vreapp/vl/openlab'. The page features the LifeWatch ERIC logo and a navigation menu with 'Home' and 'About'. A sidebar on the left indicates the user is logged in as 'Gabriel Pelouze' and provides a '[Logout]' link. The main content area is titled 'NaaVRE Open Lab' and includes the text 'Open experimentation with virtual labs'. Below this, there is a section titled 'Instances' showing '2 instances' and two user names: 'Gabriel Pelouze' and 'Spiros Koulouzis'. A checkbox labeled 'Hide my instance from this list' is present. A blue button labeled 'Launch my instance' is highlighted with a hand cursor. The bottom section is titled 'Assets' and includes a 'Workflow runs' button, 'Data Products', and 'Geographic data products'. A blue button with a refresh icon is also visible. The footer indicates '0 workflow runs'.

NaaVRE PaaS

new.demo.naavre.net/vreapp/vl/openlab

LifeWatch ERIC

Home

About

Logged in as Gabriel Pelouze [Logout]

NaaVRE Open Lab

Open experimentation with virtual labs

Instances

2 instances

Gabriel Pelouze Spiros Koulouzis

☐ Hide my instance from this list

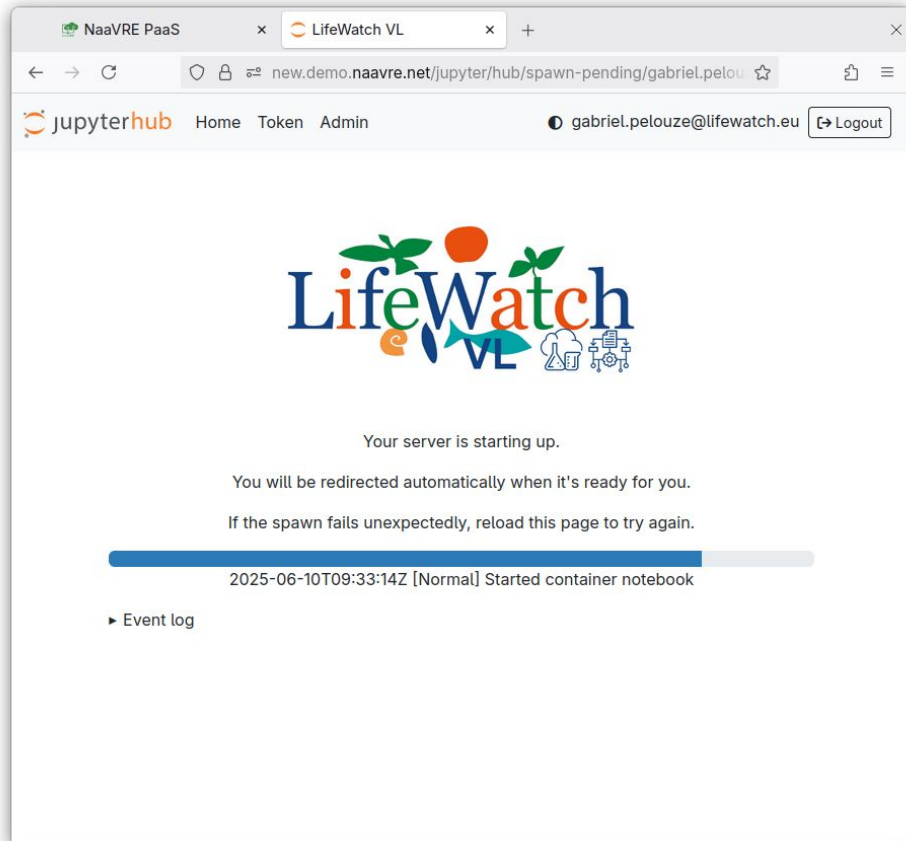
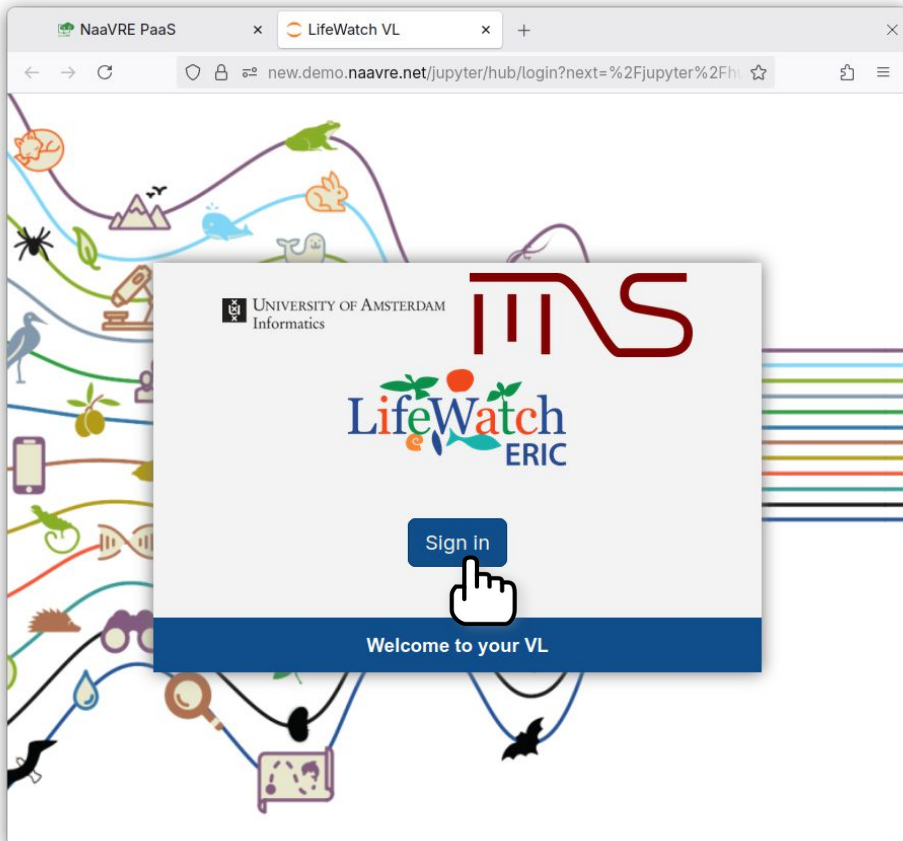
Launch my instance

Assets

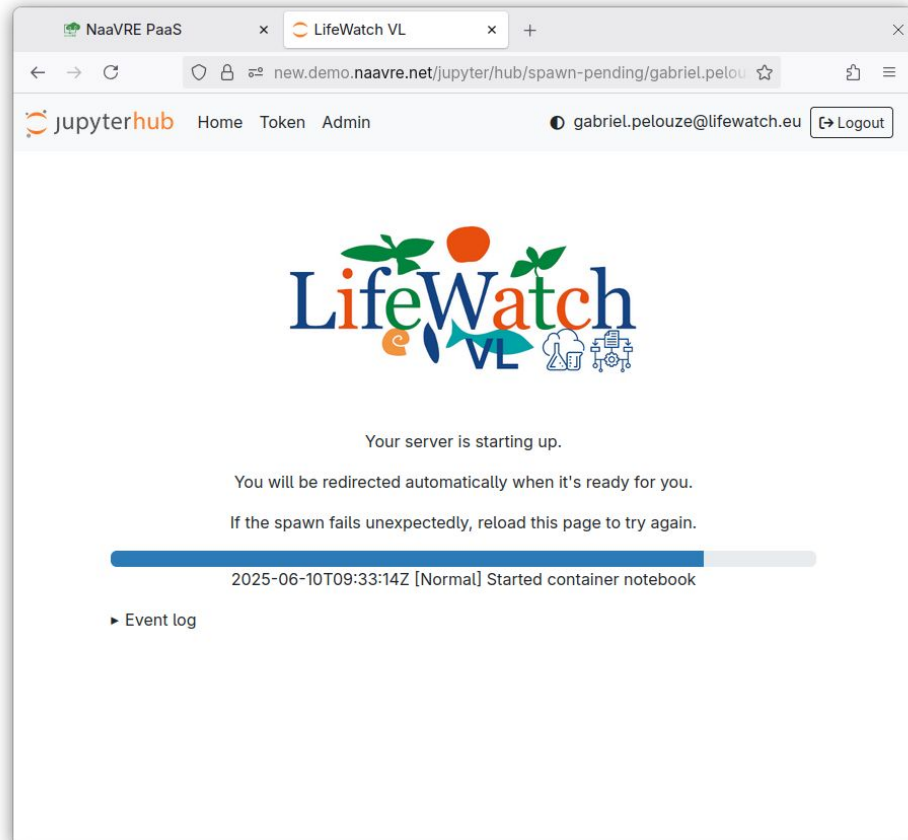
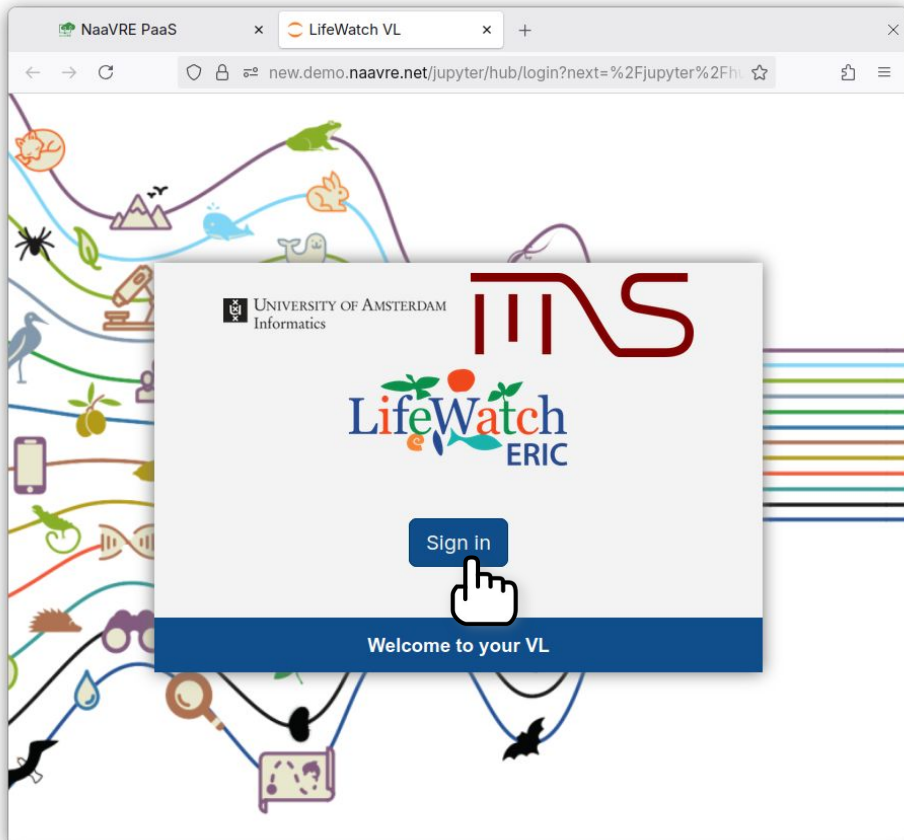
Workflow runs Data Products Geographic data products

0 workflow runs

Pick your collaborative virtual labs



Start your virtual lab

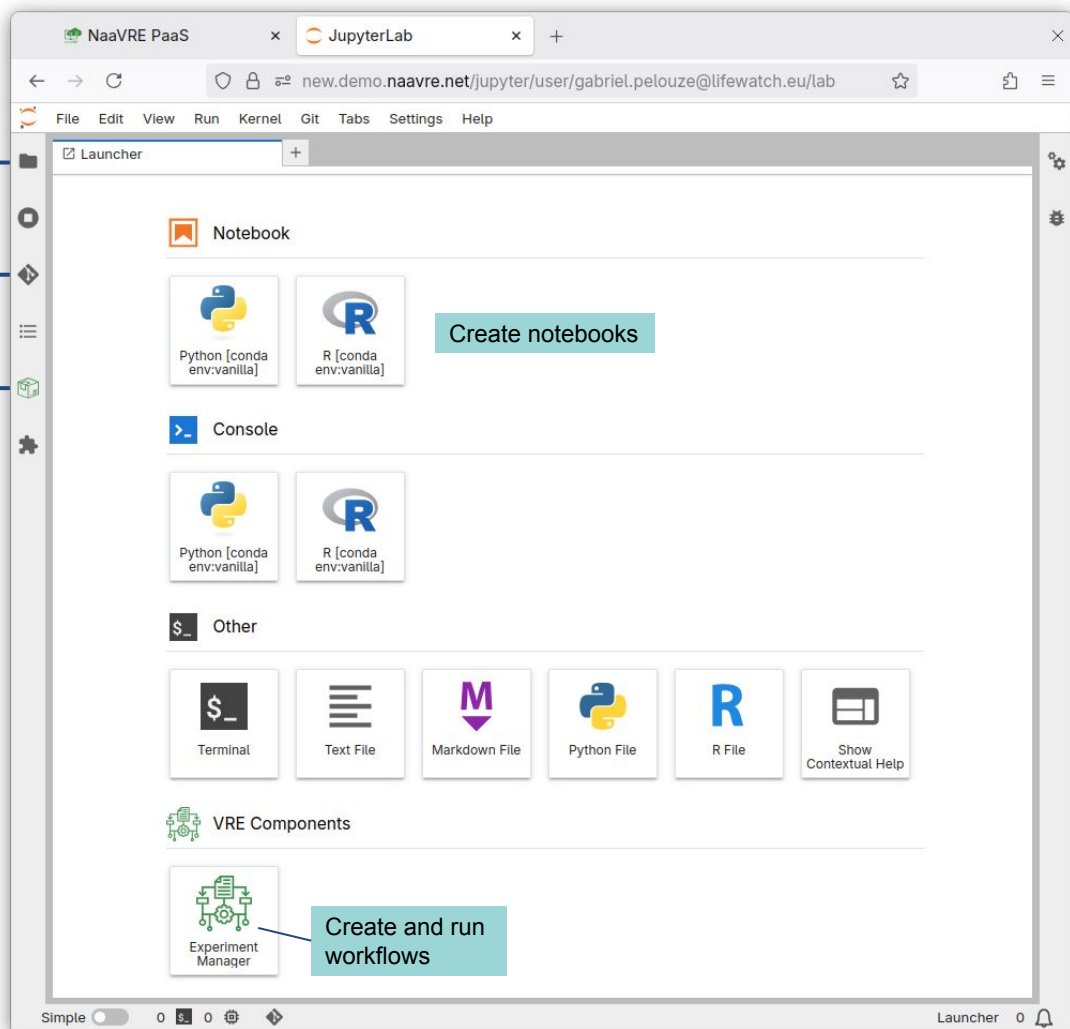


The NaaVRE interface

Manage local files

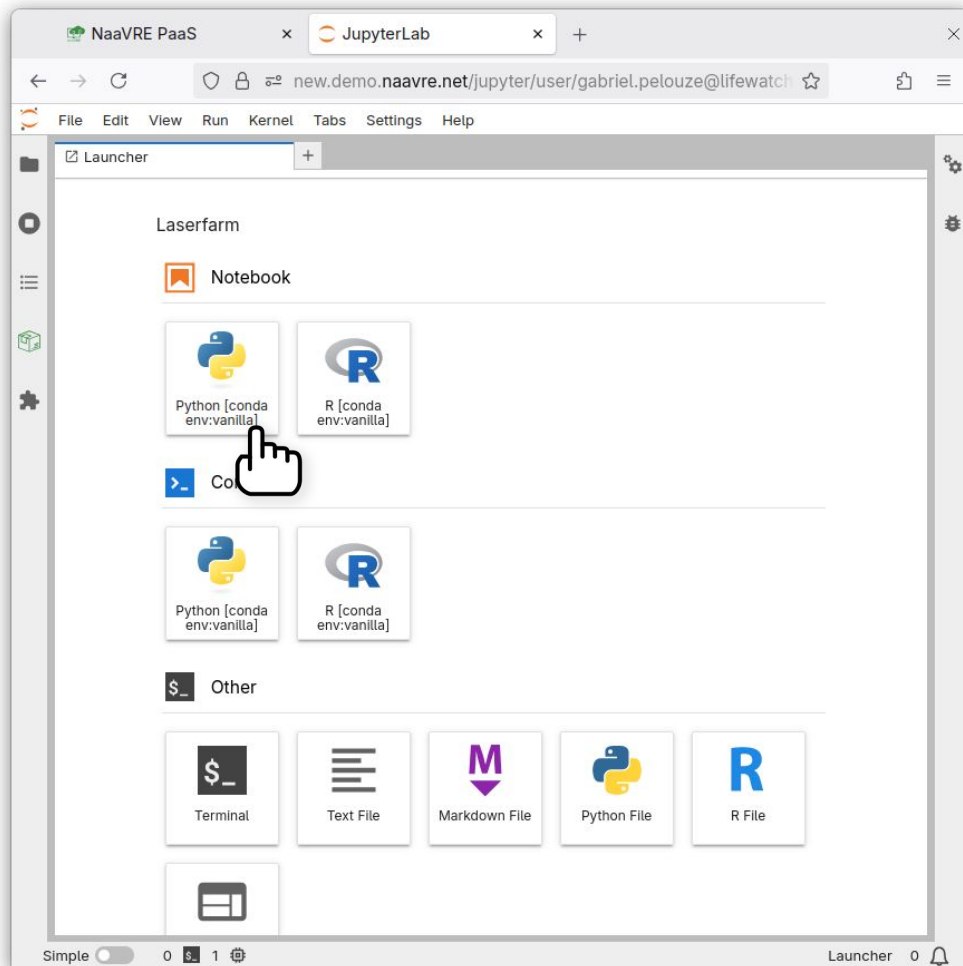
Manage your work with Git

Containerize cells



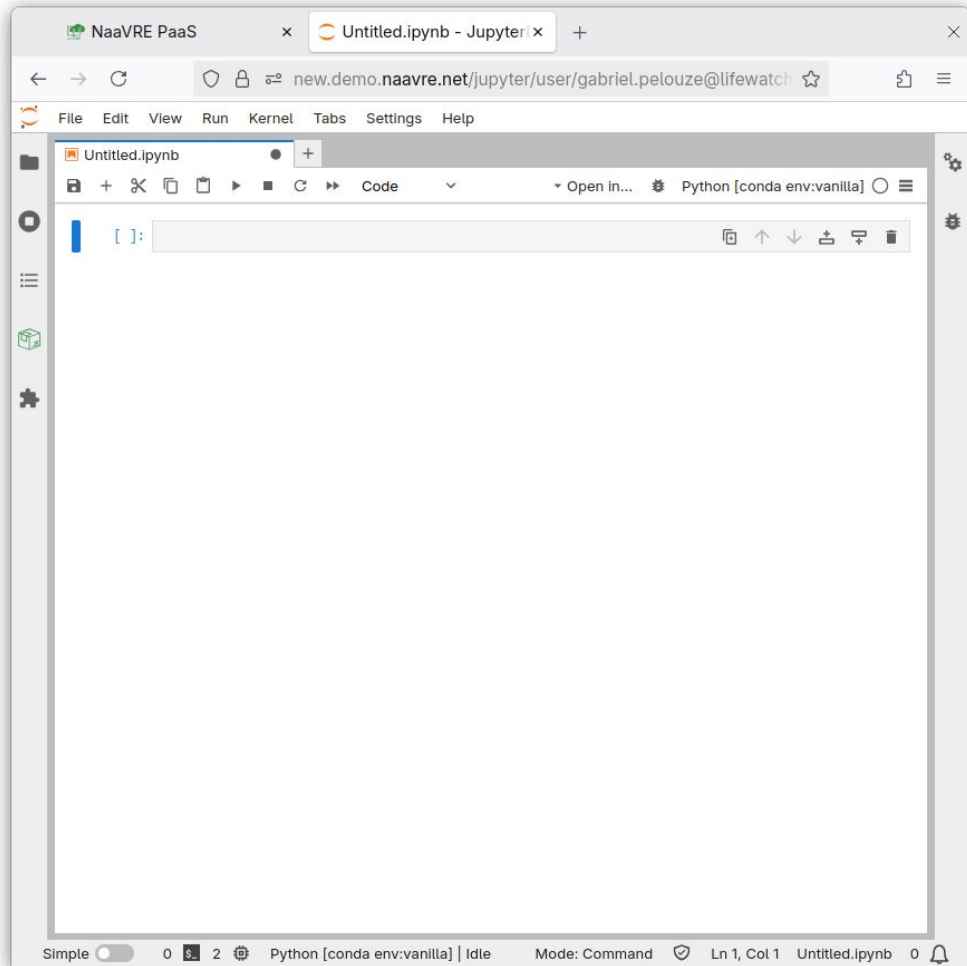
Create a notebook

1. Create a new notebook



Create a notebook

1. Create a new notebook



Create a notebook

1. Create a new notebook
2. Write some code

In Python

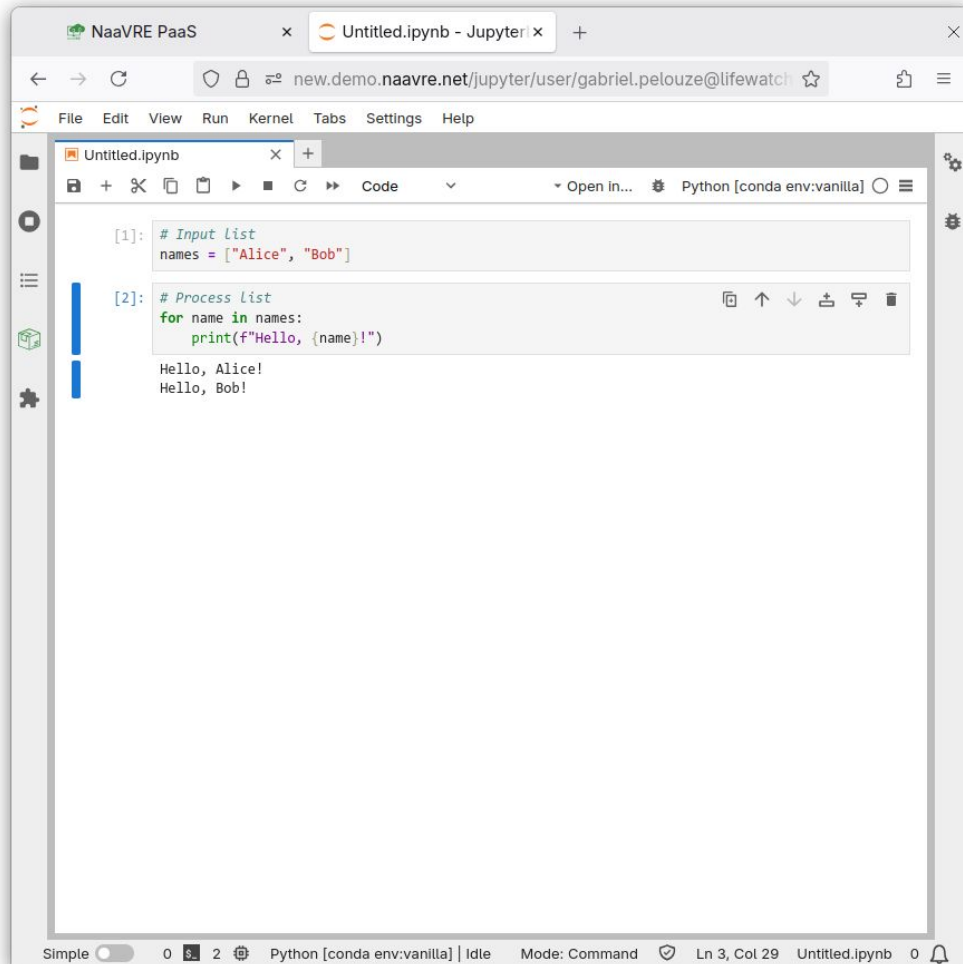
```
# Input List
names = ["Alice", "Bob"]
```

```
# Process List
for name in names:
    print(f"Hello, {name}!")
```

In R

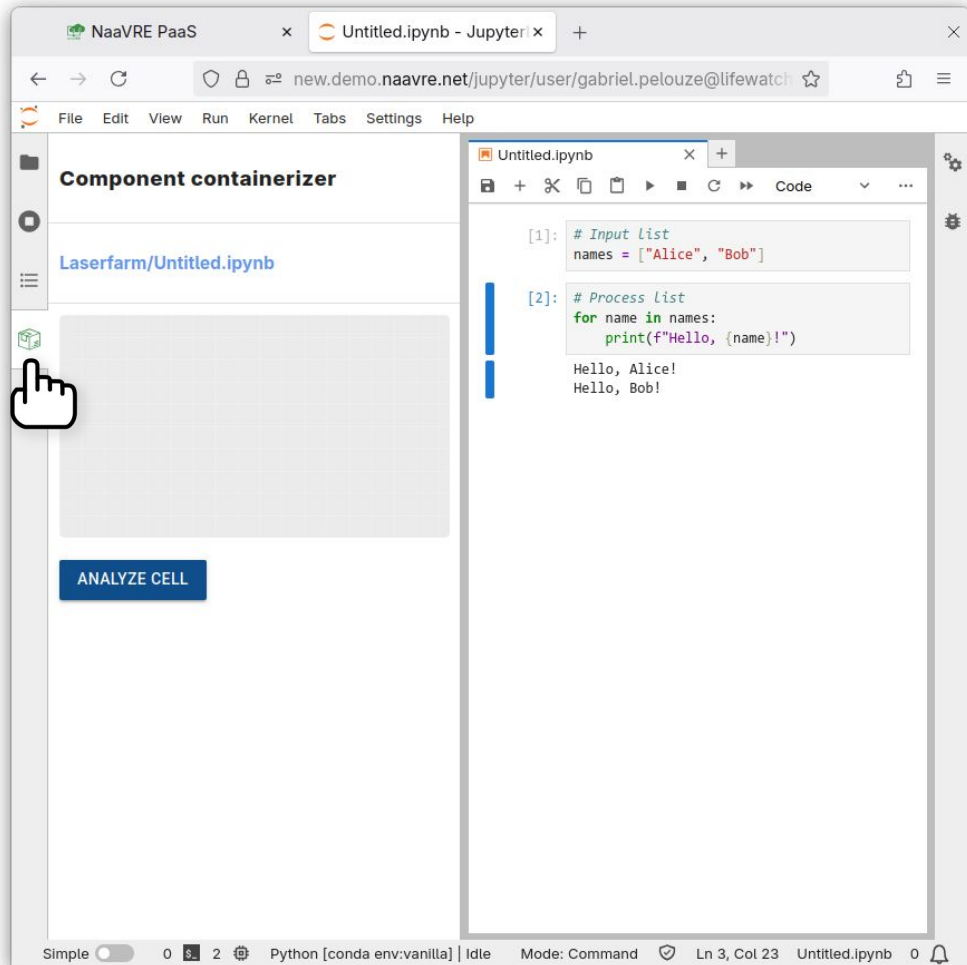
```
# Input List
names = list("Alice", "Bob")
```

```
# Process List
for (name in names) {
    print(sprintf("Hello, %s!", name))
}
```



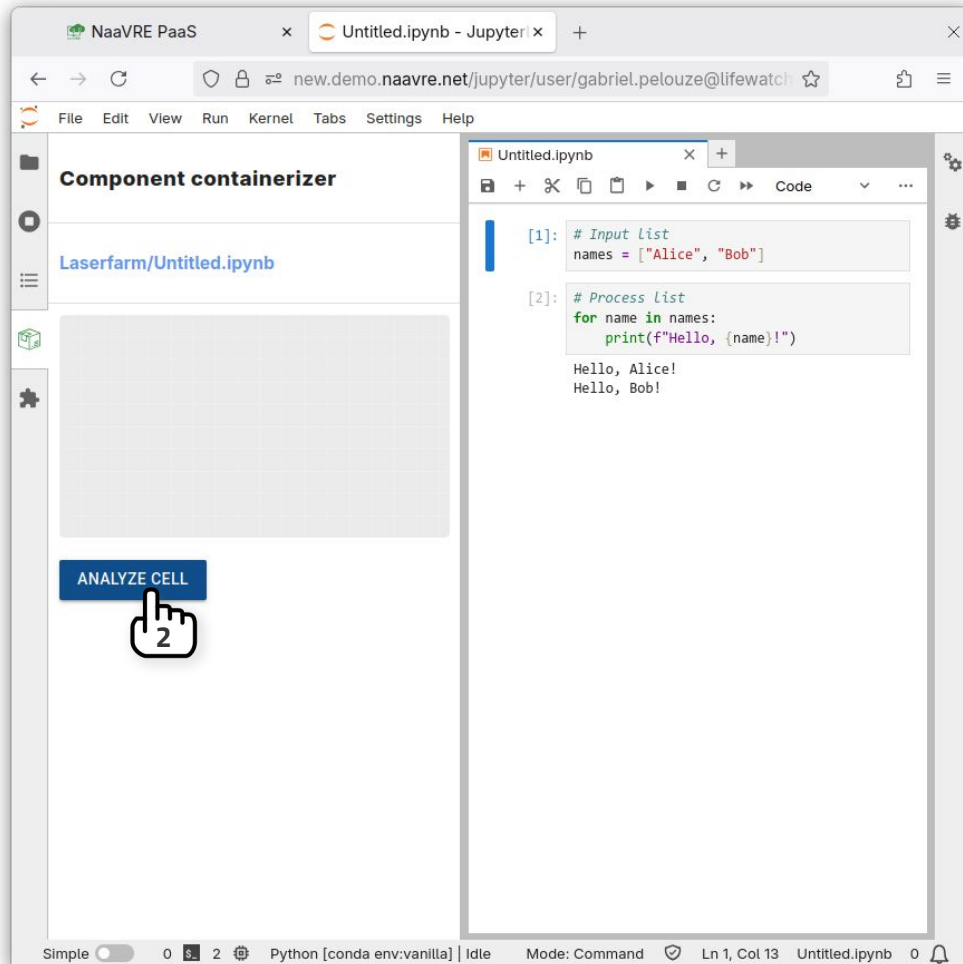
Create a notebook

1. Create a new notebook
2. Write some code
3. Containerize the cells
 - a. open the component containerizer



Create a notebook

1. Create a new notebook
2. Write some code
3. Containerize the cells
 - a. open the component containerizer
 - b. select the cell you want to containerize and click on "Analyze Cell"



Create a notebook

1. Create a new notebook
2. Write some code
3. Containerize the cells
 - a. open the component containerizer
 - b. select the cell you want to containerize
 - c. if needed, adjust the variable types

In R

List

In Python

List (set automatically)

The screenshot shows the NaaVRE PaaS interface with a Jupyter notebook titled 'Untitled.ipynb'. The notebook contains two code cells. The first cell is an input list: `[1]: # Input List
names = ["Alice", "Bob"]`. The second cell is a process list: `[2]: # Process List
for name in names:
 print(f"Hello, {name}!")`. The output of the second cell is displayed as 'Hello, Alice!' and 'Hello, Bob!'. On the left sidebar, the 'ANALYZE CELL' button is visible. Below it, the 'Outputs' section shows a variable named 'names'. A dropdown menu is open, showing options for variable types: Integer, Float, String, and List. A hand cursor is pointing at the 'List' option. At the bottom of the sidebar, there is a 'CONTAINERIZE' button and a 'Force recontainerization' checkbox.

Create a notebook

1. Create a new notebook
2. Write some code
3. Containerize the cells
 - a. open the component containerizer
 - b. select the cell you want to containerize
 - c. if needed, adjust the variable types
 - d. select the base image

In R

r

In Python

python

The screenshot shows the NaaVRE PaaS interface. On the left, a sidebar displays a file explorer with 'Laserfarm/Untitled.ipynb'. Below it, a preview of the notebook shows a code cell with the variable 'names' assigned a list of strings. A blue 'ANALYZE CELL' button is visible. Below the button, a dropdown menu lists available base images: 'vanilla', 'python', 'r', 'biodyt-hackathon25', and 'laserfarm'. A hand cursor is pointing at the 'python' option. At the bottom of this menu is a 'CONTAINERIZE' button. Below the menu, there is a checkbox for 'Force recontainerization' which is currently unchecked. On the right, the Jupyter notebook editor is open, showing two code cells. The first cell is an input list:

```
[1]: # Input List
names = ["Alice", "Bob"]
```

. The second cell is a process list:

```
[2]: # Process List
for name in names:
    print(f"Hello, {name}!")
```

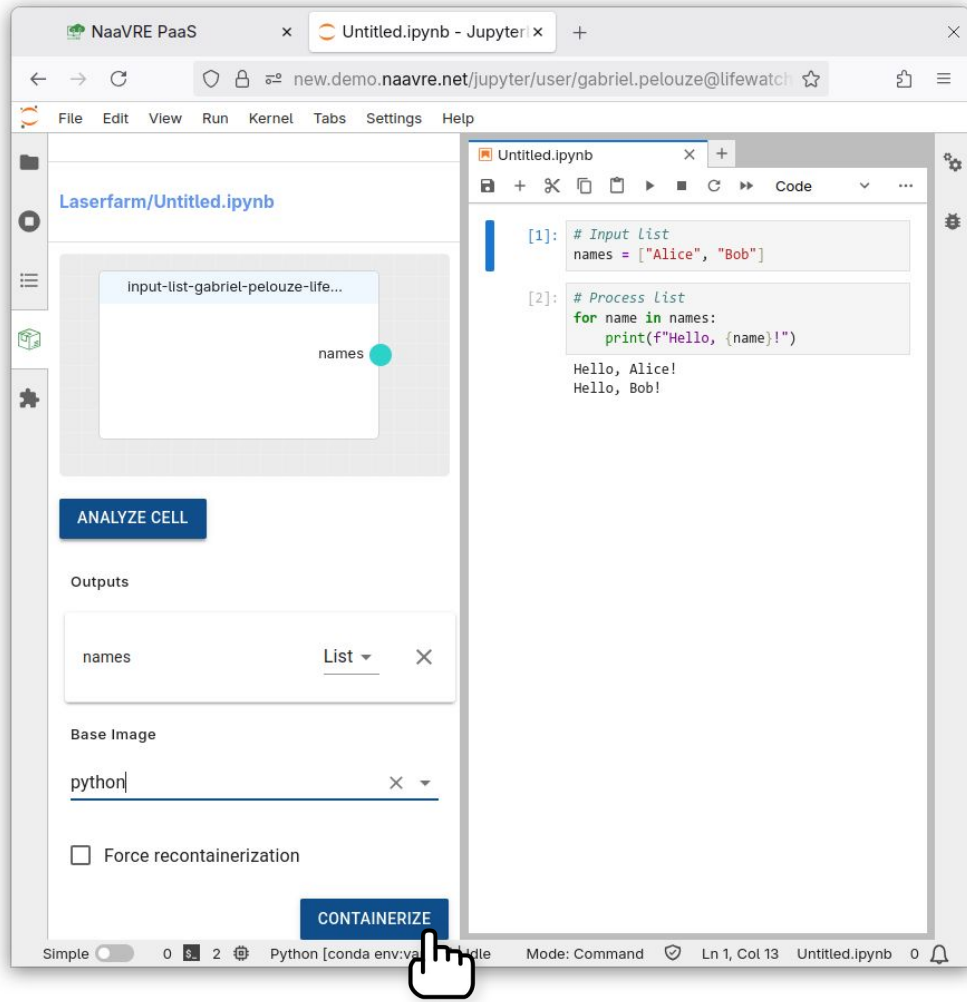
. The output of the second cell is visible:

```
Hello, Alice!
Hello, Bob!
```

. The top of the interface shows the browser address bar with the URL 'new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch' and the NaaVRE PaaS logo.

Create a notebook

1. Create a new notebook
2. Write some code
3. Containerize the cells
 - a. open the component containerizer
 - b. select the cell you want to containerize
 - c. if needed, adjust the variable types
 - d. select the base image
 - e. containerize the cell



The screenshot displays the NaaVRE PaaS interface. On the left, a sidebar shows a file explorer with 'Laserfarm/Untitled.ipynb'. The main area shows a preview of the notebook cell, with a variable 'names' highlighted. Below the preview, there is an 'ANALYZE CELL' button. Underneath, the 'Outputs' section shows the variable 'names' as a 'List'. The 'Base Image' section has a dropdown menu set to 'python'. At the bottom, there is a checkbox for 'Force recontainerization' and a 'CONTAINERIZE' button. On the right, the Jupyter notebook editor is open, showing two code cells. The first cell defines a list 'names' with 'Alice' and 'Bob'. The second cell is a process list that iterates over 'names' and prints 'Hello, {name}!'. The output of the second cell shows 'Hello, Alice!' and 'Hello, Bob!'. A hand cursor is pointing at the 'CONTAINERIZE' button.

NaaVRE PaaS x Untitled.ipynb - Jupyter x +

new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch

File Edit View Run Kernel Tabs Settings Help

Laserfarm/Untitled.ipynb

input-list-gabriel-pelouze-life...

names

ANALYZE CELL

Outputs

names List X

Base Image

python X

☐ Force recontainerization

CONTAINERIZE

```
[1]: # Input List
names = ["Alice", "Bob"]

[2]: # Process List
for name in names:
    print(f"Hello, {name}!")

Hello, Alice!
Hello, Bob!
```

Simple 0 2 Python [conda env:va] Mode: Command Ln 1, Col 13 Untitled.ipynb 0

Create a notebook

1. Create a new notebook
2. Write some code
3. Containerize the cells
 - a. open the component containerizer
 - b. select the cell you want to containerize
 - c. if needed, adjust the variable types
 - d. select the base image
 - e. containerize the cell
 - f. well done!
 - g. repeat steps b–e for other cells

The screenshot displays the NaaVRE PaaS web interface. The top navigation bar includes 'File', 'Edit', 'View', 'Run', 'Kernel', 'Tabs', 'Settings', and 'Help'. The main area is split into two panes. The left pane, titled 'Laserfarm/Untitled.ipynb', shows a visual representation of a Jupyter notebook cell with a variable 'names' and a blue 'ANALYZE CELL' button. Below this, the 'Outputs' section shows the variable 'names' as a 'List'. The 'Base Image' is set to 'python', and there is a checkbox for 'Force recontainerization'. A blue 'CONTAINERIZE' button is at the bottom right of this pane. The right pane shows the raw code of the notebook cell:

```
[1]: # Input List
names = ["Alice", "Bob"]

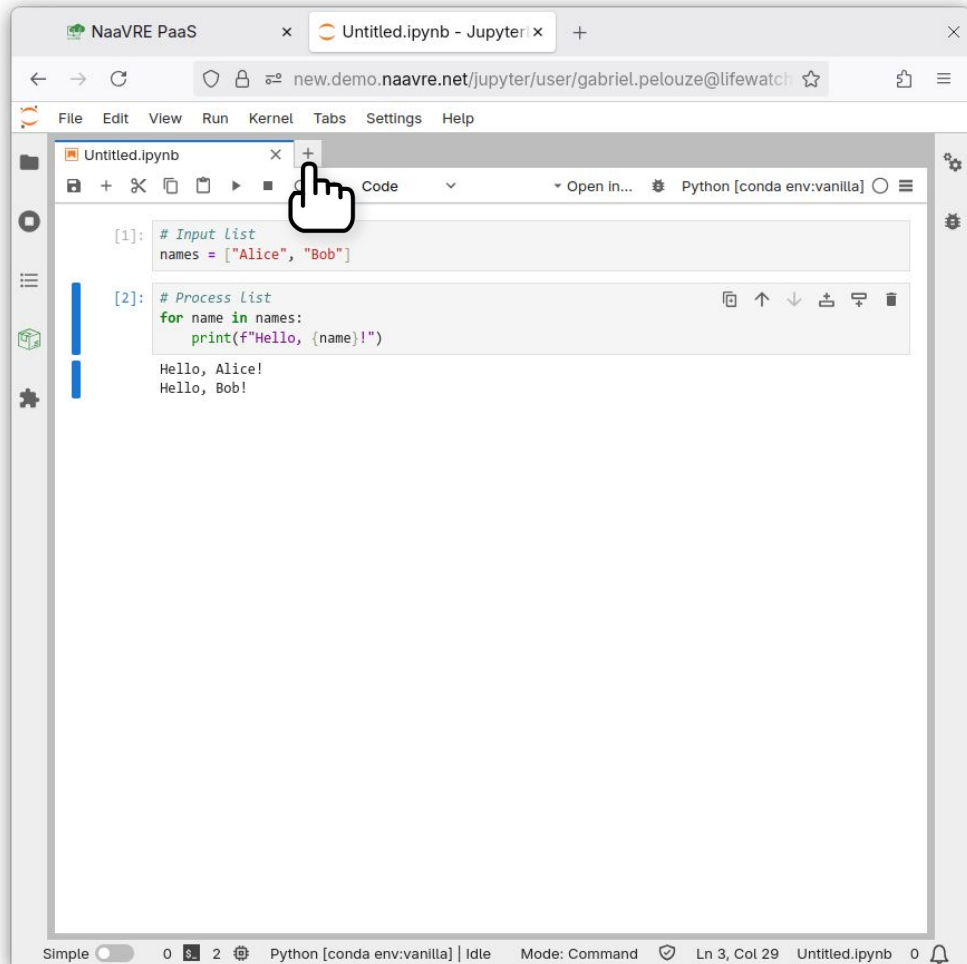
[2]: # Process List
for name in names:
    print(f"Hello, {name}!")

Hello, Alice!
Hello, Bob!
```

 At the bottom right, two green notification boxes indicate successful actions: 'Added cell input-list-gabriel-pelouze-lifewatch-eu to the catalogue' and 'Created cell Input-list-gabriel-pelouze-lifewatch-eu'. The status bar at the very bottom shows 'Simple' mode, '0' errors, '2' warnings, 'Python [conda env:vanilla]', 'Idle' mode, and 'Ln 1, Col 13'.

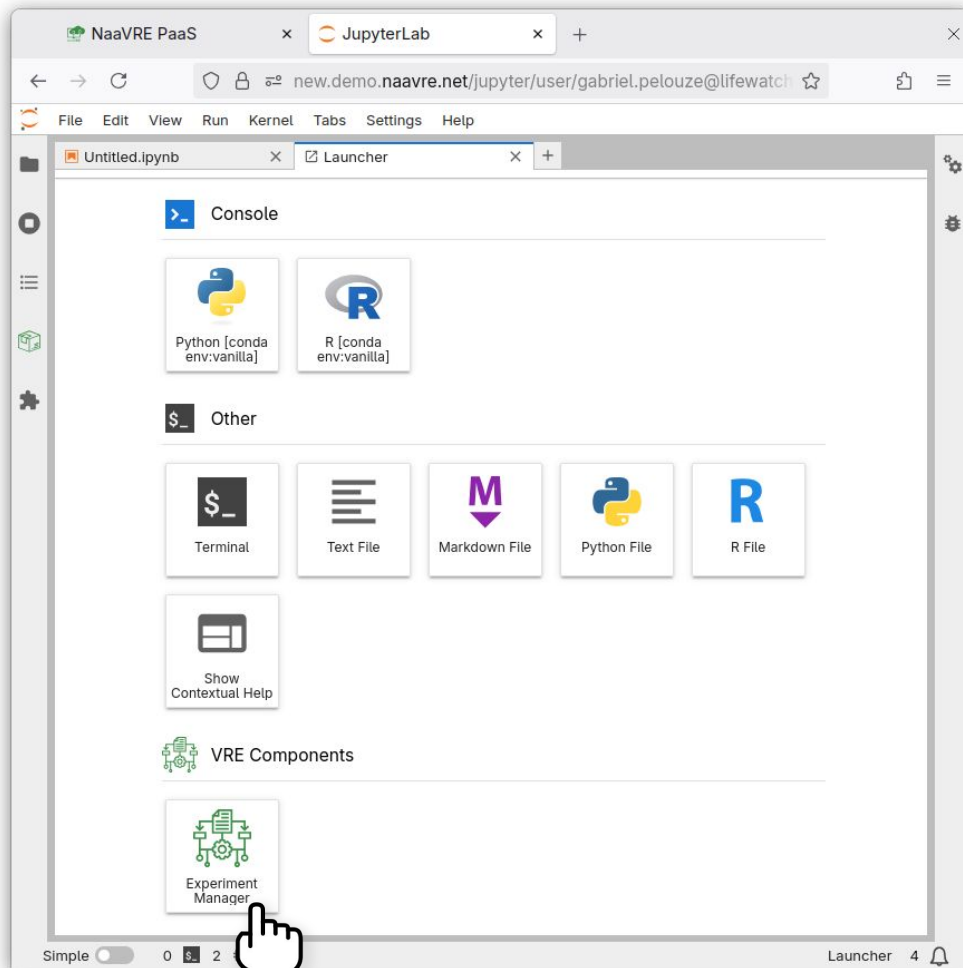
Create a workflow

1. Open the experiment manager



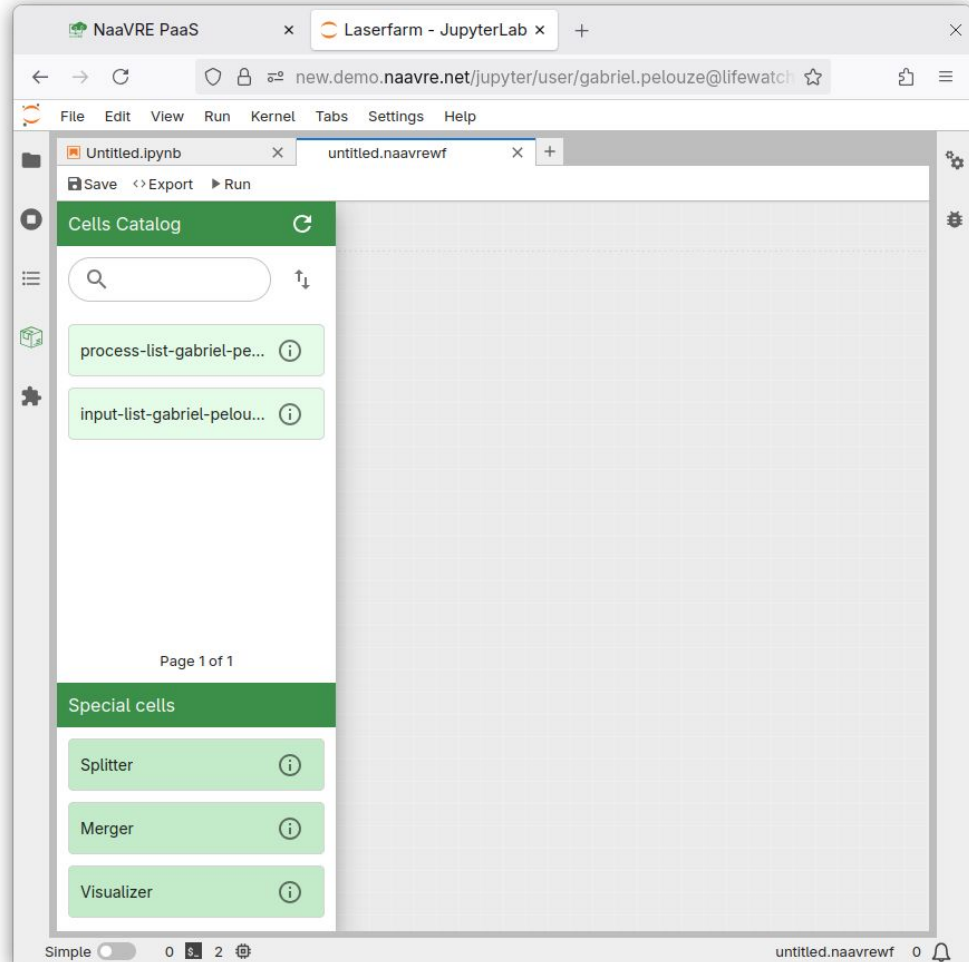
Create a workflow

1. Open the experiment manager



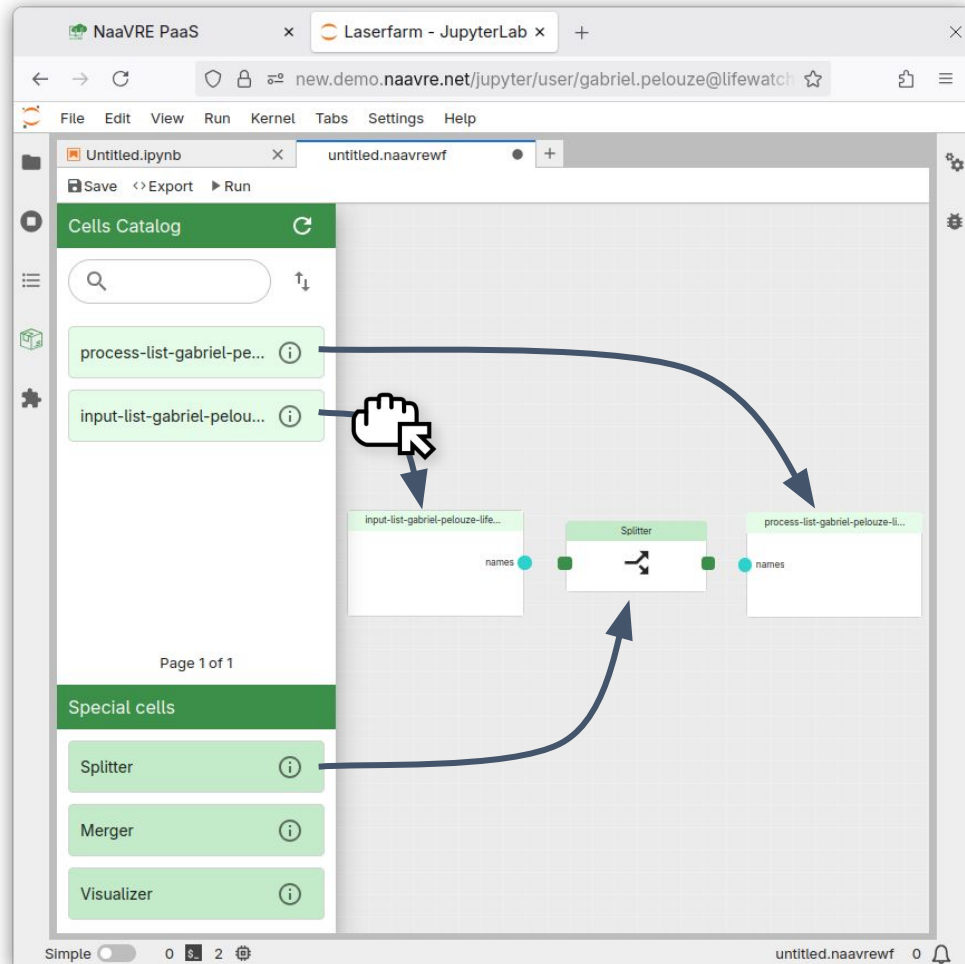
Create a workflow

1. Open the experiment manager



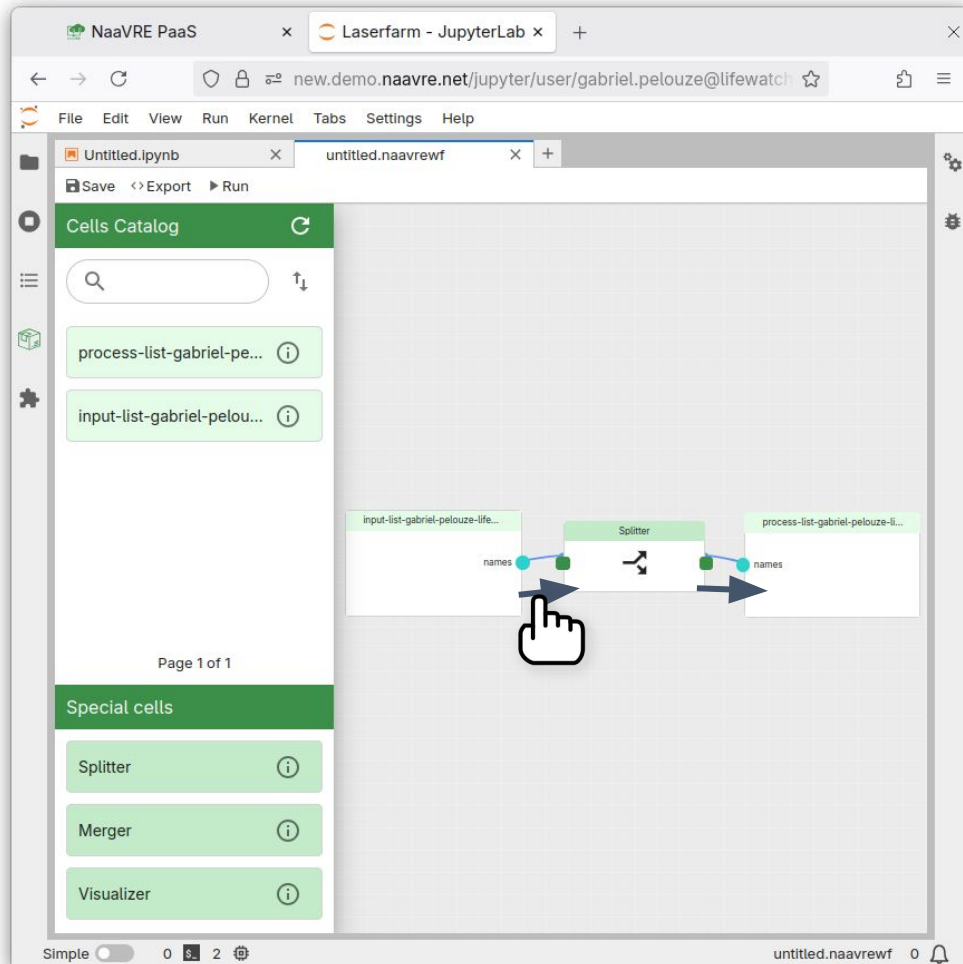
Create a workflow

1. Open the experiment manager
2. Drag and drop the cells onto the canvas



Create a workflow

1. Open the experiment manager
2. Drag and drop the cells onto the canvas
3. Connect the cells



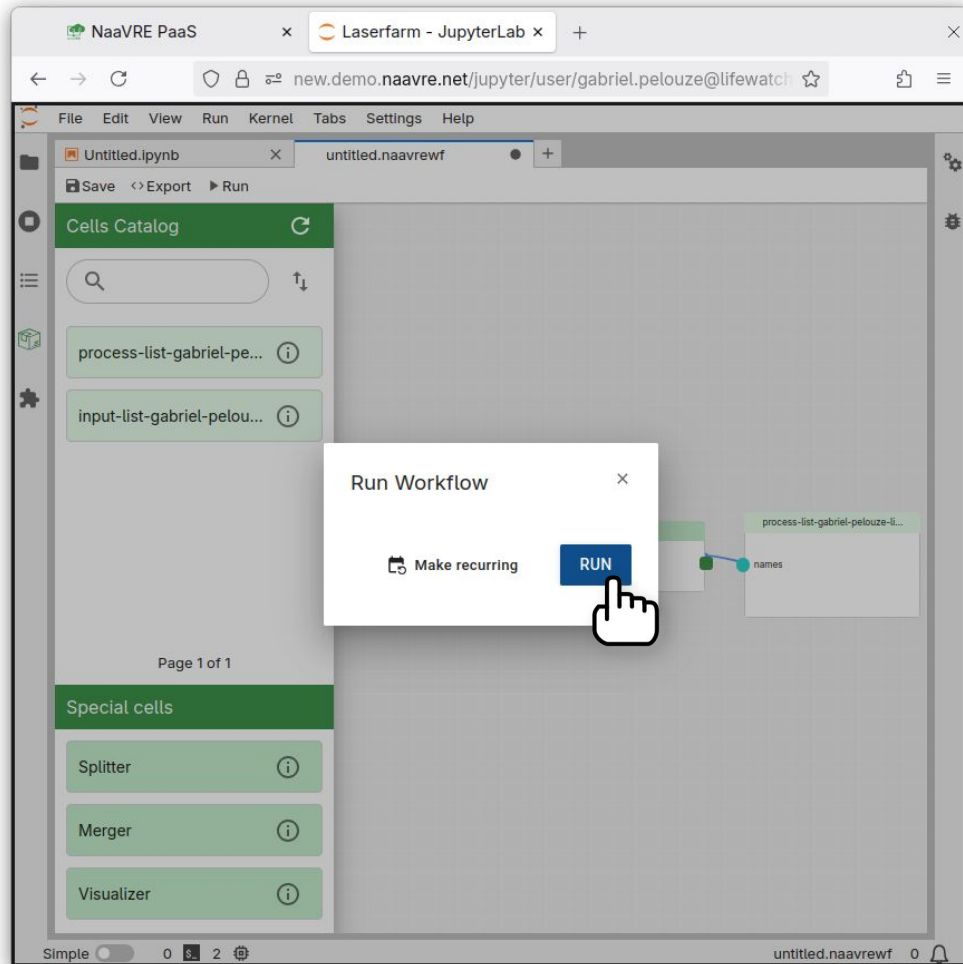
Create a workflow

1. Open the experiment manager
2. Drag and drop the cells onto the canvas
3. Connect the cells
4. Execute the workflow

The screenshot displays the NaaVRE PaaS web interface. The browser address bar shows the URL `new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch`. The interface includes a menu bar with options: File, Edit, View, Run, Kernel, Tabs, Settings, and Help. Below the menu, there are tabs for 'Untitled.ipynb' and 'untitled.naavrewf'. A 'Cells Catalog' panel on the left lists available cells: 'process-list-gabriel-pe...', 'input-list-gabriel-pelou...', and 'Special cells' (containing 'Splitter', 'Merger', and 'Visualizer'). A hand icon is shown dragging a cell from the catalog to the main canvas. The canvas displays a workflow diagram with three cells: 'input-list-gabriel-pelouze-life...', 'Splitter', and 'process-list-gabriel-pelouze-li...'. The 'input' cell is connected to the 'Splitter', which is then connected to the 'process' cell. The status bar at the bottom indicates 'Simple' mode, a progress bar with '0' and '2' markers, and the filename 'untitled.naavrewf'.

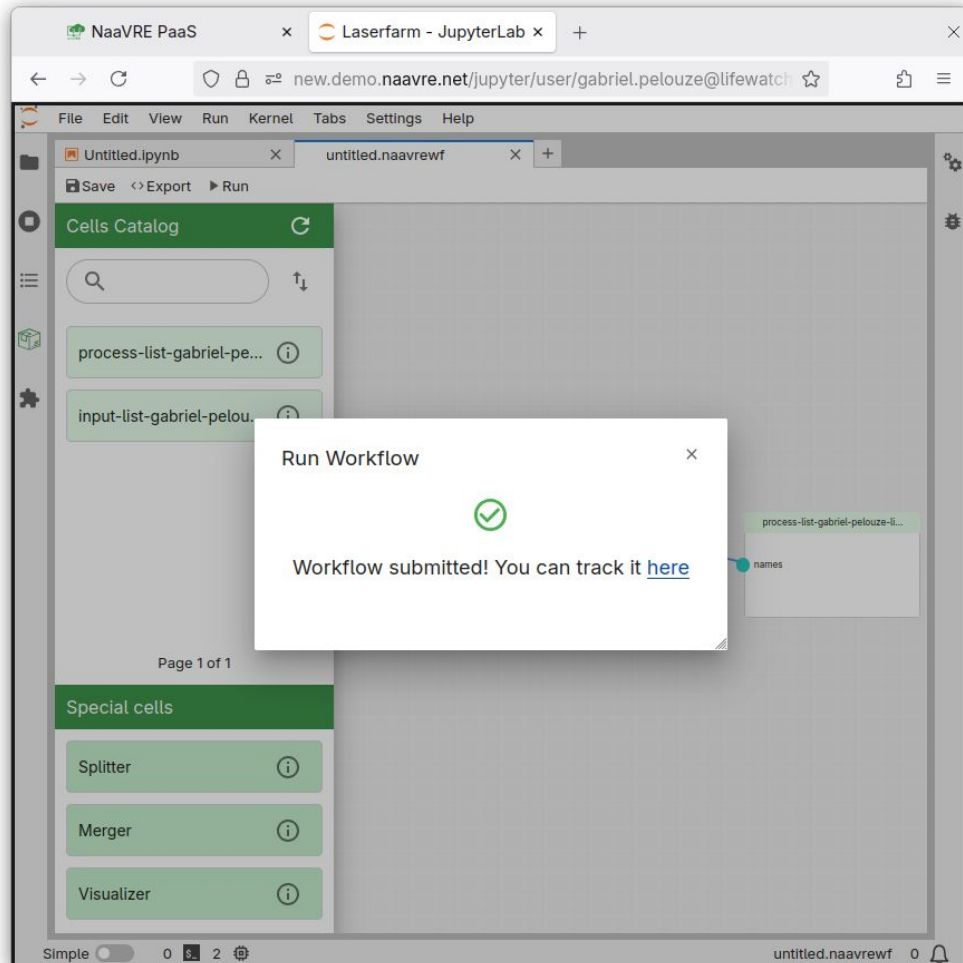
Create a workflow

1. Open the experiment manager
2. Drag and drop the cells onto the canvas
3. Connect the cells
4. Execute the workflow



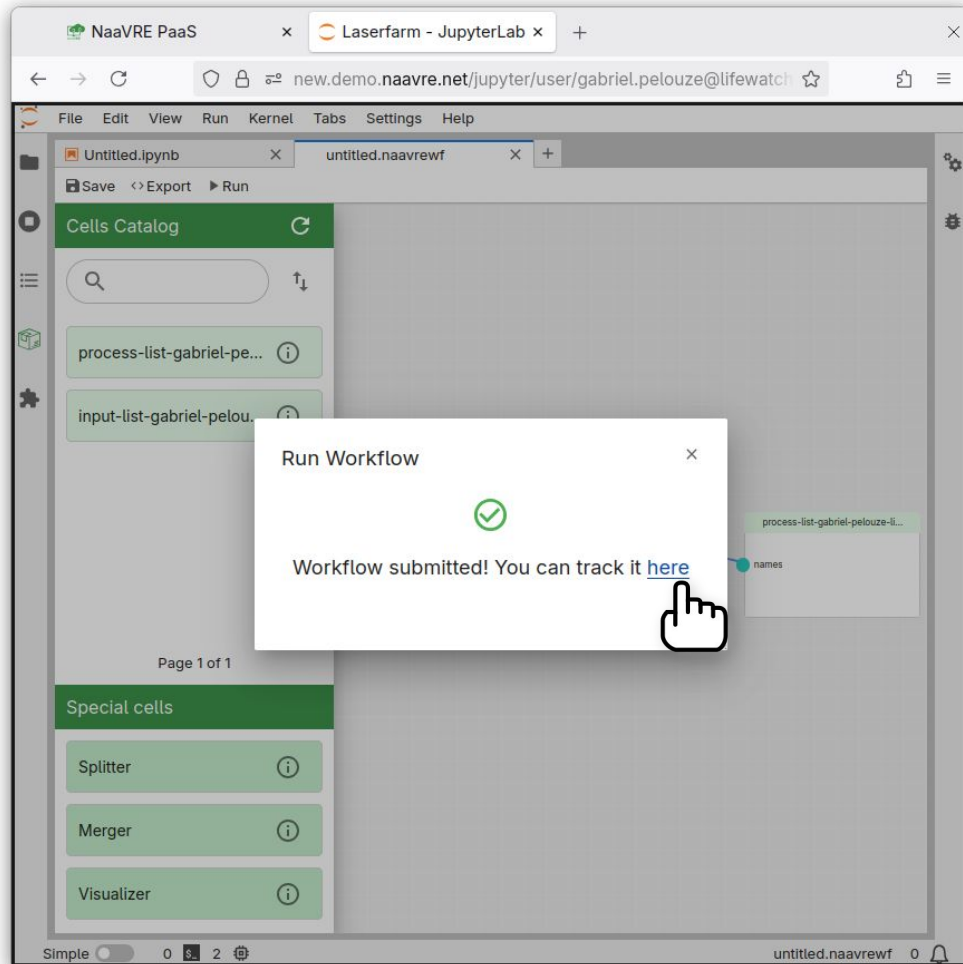
Create a workflow

1. Open the experiment manager
2. Drag and drop the cells onto the canvas
3. Connect the cells
4. Execute the workflow
5. Well done!



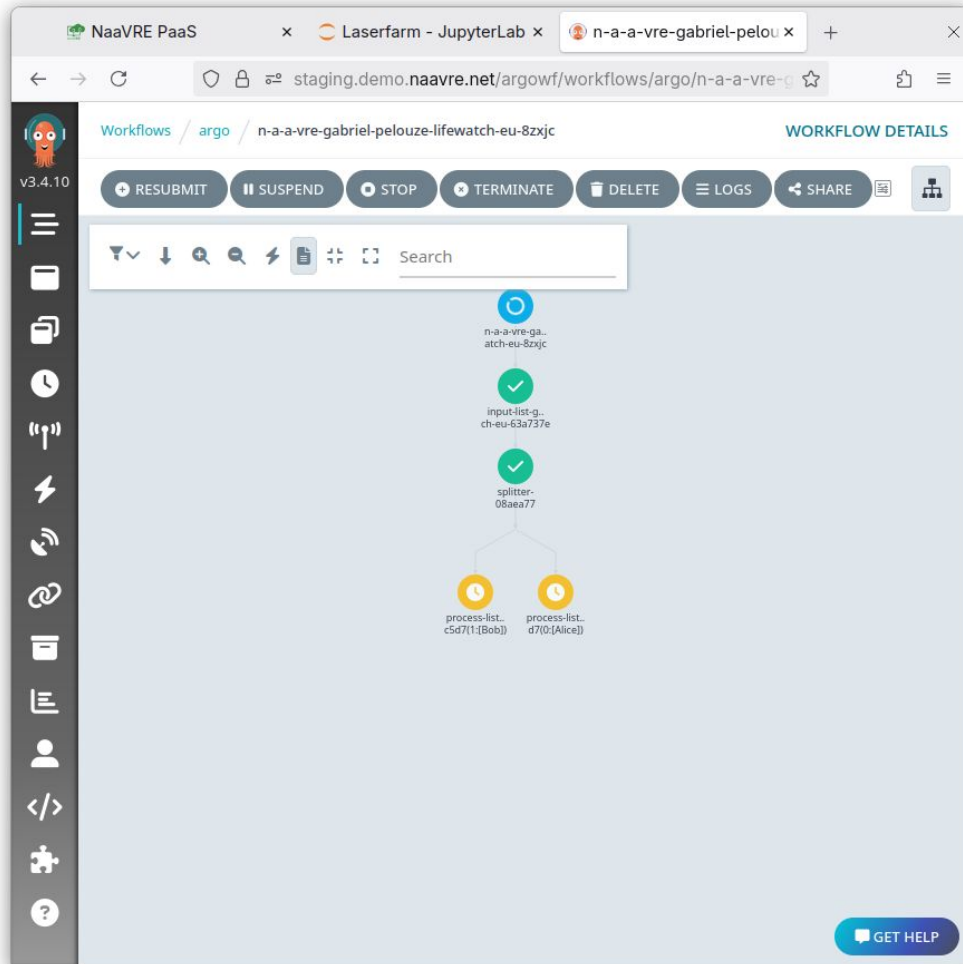
Monitor a workflow

1. Click on the link to open the workflow manager, Argo
2. If needed, log in to argo



Monitor a workflow

1. Click on the link to open the workflow manager, Argo
2. If needed, log in to argo
3. Check your workflow status



Exercises

Start the **Open Lab** and the exercises in `Open Lab/Git public/exercises/` :

- Exercise 1: Workflow parameters and secrets
- Exercise 2: Splitter and merger to create parallel workflows
- Exercise 3: File management

The screenshot shows the NaaVRE PaaS interface with a browser window open to `new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch.eu/lab/tree/Open Lab / Git public / exercises /`. The left sidebar displays a file tree with the following items: `Exercise 1 params and secrets.ipynb`, `Exercise 2 split and merge.ipynb` (selected), `Exercise 3 file management.ipynb`, `Solution 1.ipynb`, `Solution 1.naavrewf`, `Solution 2.ipynb`, `Solution 2.naavrewf`, `Solution 3.ipynb`, and `Solution 3.naavrewf`. The main area shows the 'Exercise 2: Splitter and merger' notebook. The title is 'Exercise 2: Splitter and merger'. The text describes the exercise: 'In this exercise, we learn how to use the splitter and merger. This is useful to process data in parallel with the workflow. We start with the tutorial workflow (Your first workflow in Python.ipynb), and modify it to add the merger. The cells are copied in this notebook, so that you can modify them directly.' Below the text is a code cell with the following content:

```
[ ]: # ex2 1: input list
names = ["Alice", "Bob"]

Step 1

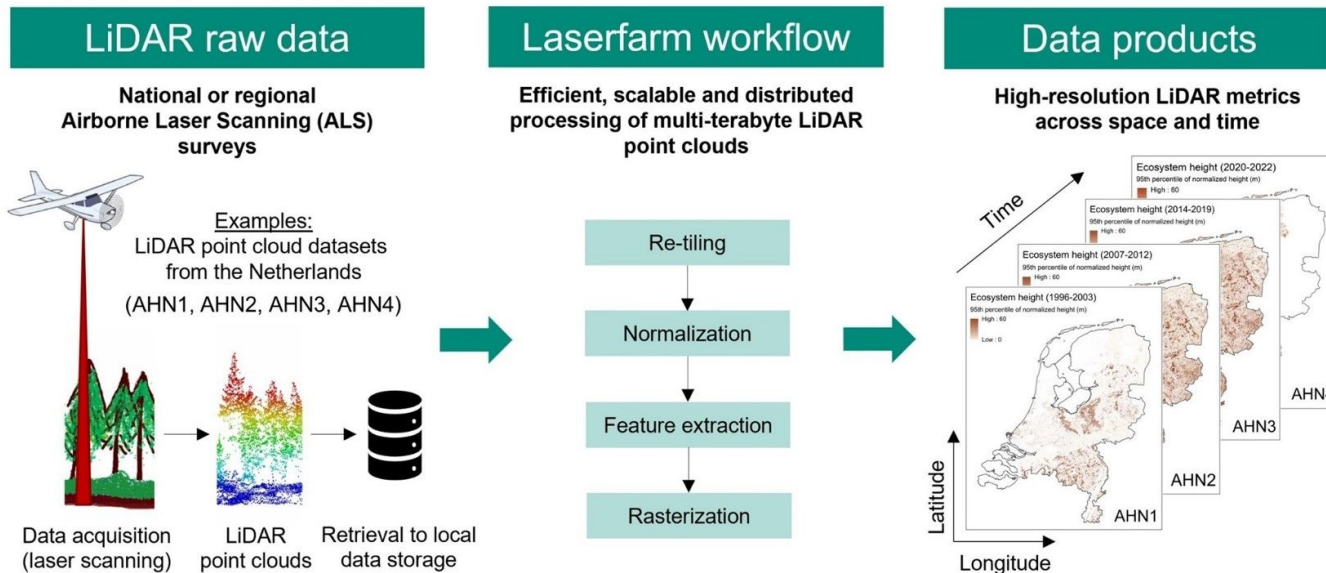
Modify cell 2 to create a variable sentences, instead of printing the message:

sentences = []
for name in names:
    sentences.append(f"Hello, {name}!")
```

The screenshot shows the NaaVRE PaaS interface with a browser window open to `new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch.eu/lab/tree/Open Lab / Git public / exercises /`. The left sidebar displays a file tree with the following items: `Exercise 1 params and secrets.ipynb`, `Exercise 2 split and merge.ipynb`, `Exercise 3 file management.ipynb`, `Solution 1.ipynb`, `Solution 1.naavrewf`, `Solution 2.ipynb`, `Solution 2.naavrewf` (selected), `Solution 3.ipynb`, and `Solution 3.naavrewf`. The main area shows the 'Solution 2.naavrewf' workflow. The title is 'Solution 2.naavrewf'. The text describes the workflow: 'Exercise 2 split and merge X'. Below the text is a 'Cells Catalog' panel with a search bar and a list of cells: `untitled-gabriel-pelouz...`, `ex3-1-create-file-gabri...`, `ex3-3-upload-file-gabr...`, `ex3-2-plot-file-gabriel...`, `ex2-3-print-list-gabriel...`, `ex2-1-input-list-gabriel...`, and `ex2-2-process-list-gab...`. The right panel shows a visual representation of the workflow, with a box labeled 'ex2-1-input-list-gpelouze' connected to a 'Splitter' box, which then branches into two parallel paths.

Laserfarm Virtual Lab

Scenario: map vegetation characteristics using LiDAR data.



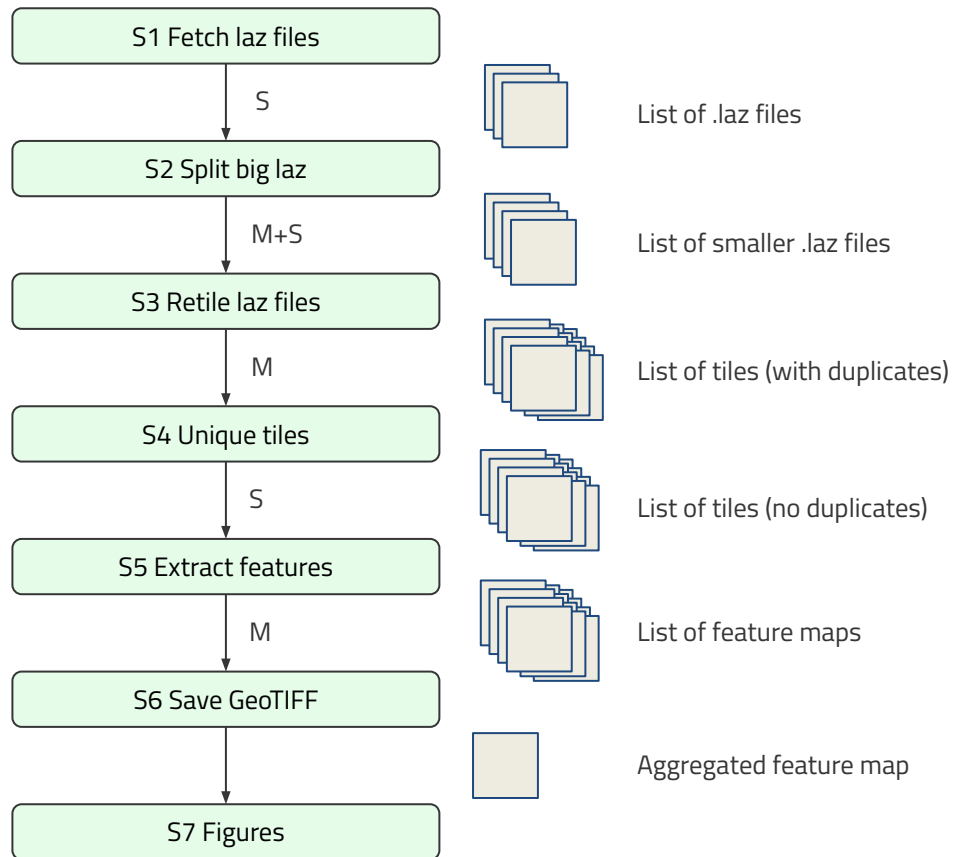
Yifang Shi



Exercise

- Start the **Laserfarm** virtual lab
- Run the notebook `Laserfarm/Git public/exercises/Laserfarm.ipynb`
Discuss the implications of processing large files in a notebook
- Containerize the cells and build a workflow
- Add splitters and mergers to parallelize the data processing. *Discuss with your classmates and tutors to figure out where to add them*

Laserfarm workflow

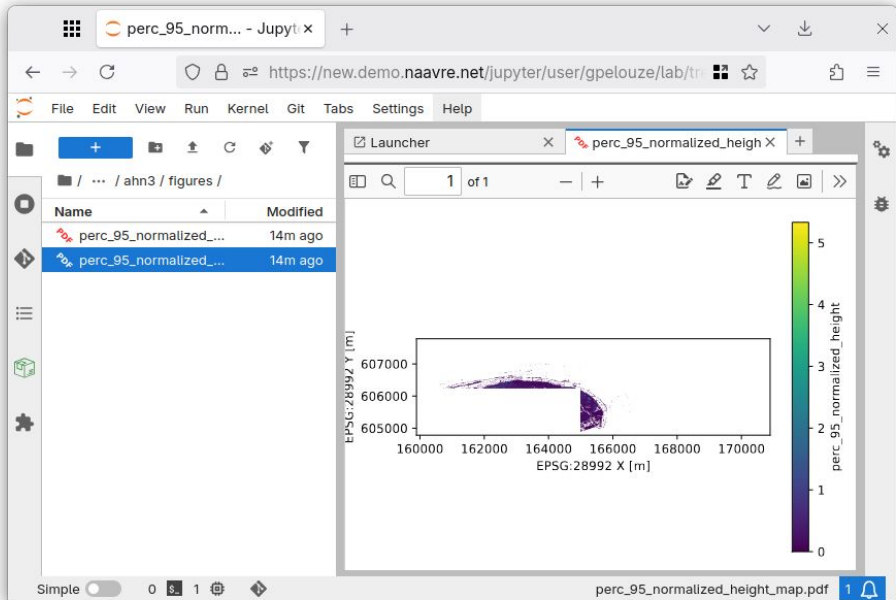


Laserfarm workflow



Laserfarm workflow results

Getting the output: open the file browser and go to:
naa-vre-user-data/v1-laserfarm/small_terschelling/ahn3/

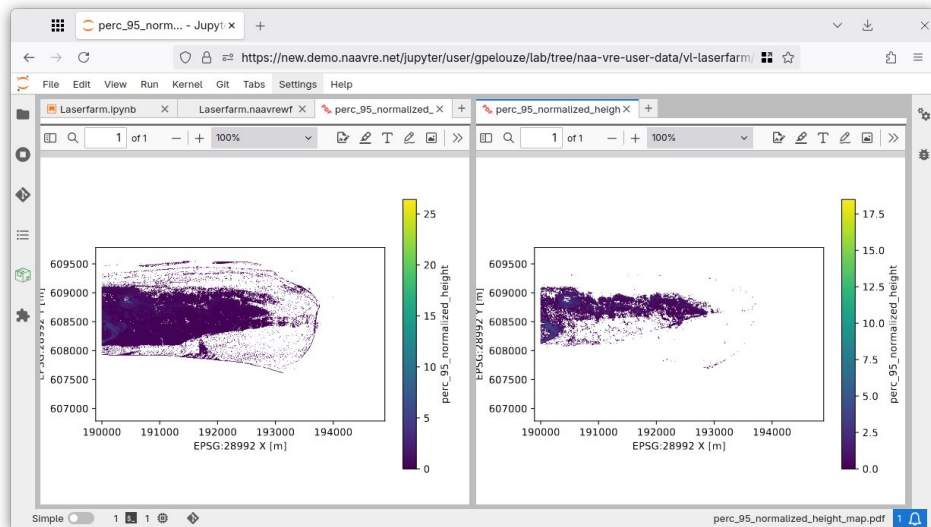


Other datasets: explore values of
param_minio_public_dataset_prefix:

v1-laserfarm / small_terschelling / ahn3 /
medium_ameland / ahn4 /

Other datasets: change value of param_feature_name

List: <https://laserchicken.readthedocs.io/en/latest/#features>





THANKS!



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Mission 4 "Education and Research" - Component 2: "From research to business" - Investment
3.1: "Fund for the realisation of an integrated system of research and innovation infrastructures"

