



# Open Science on Cloud using Jupyter Notebooks

## Cloud workflows with NaaVRE

### Concepts, tutorial and exercises

G. Pelouze, S. Koulouzis, Z. Zhao

(LifeWatch ERIC VLIC / MNS, University of Amsterdam)

25/06/2025



UNIVERSITY  
OF AMSTERDAM

**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"



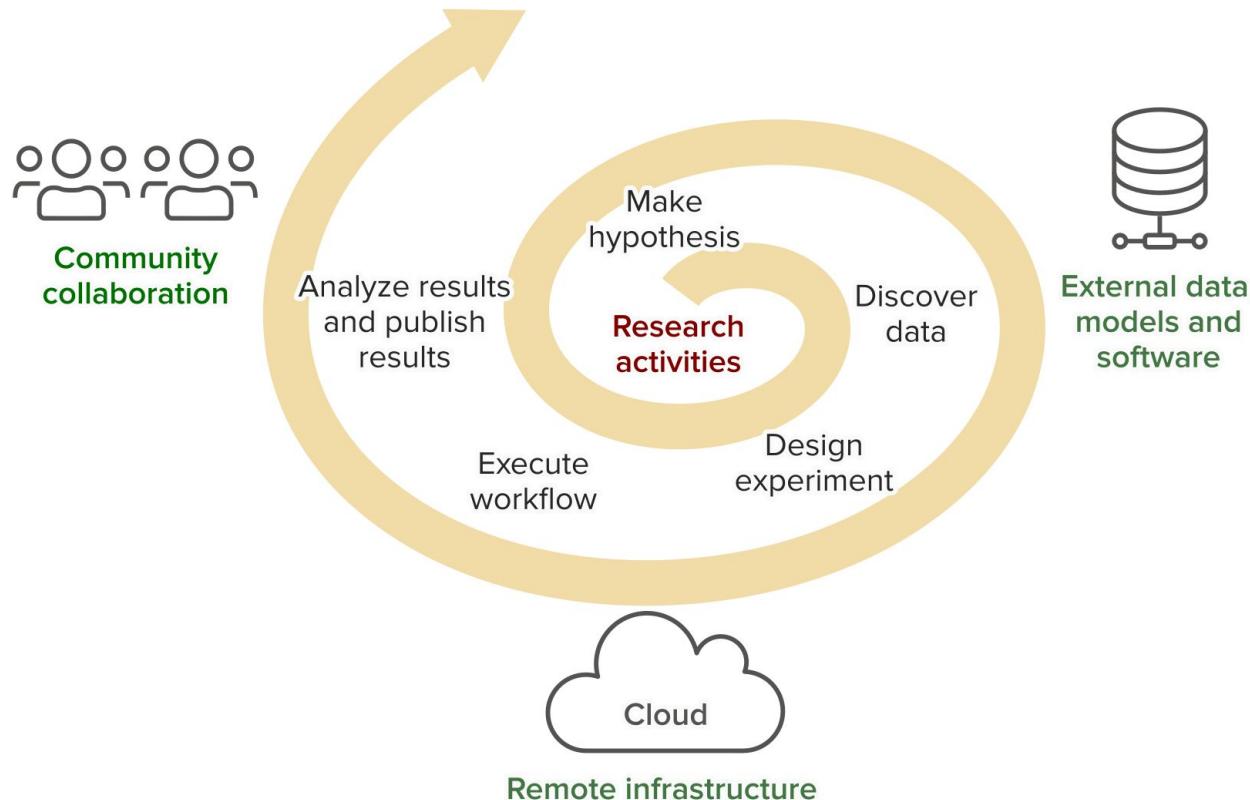
Finanziato  
dall'Unione europea  
NextGenerationEU



Ministero  
dell'Università  
e della Ricerca



# Data-centric research lifecycle



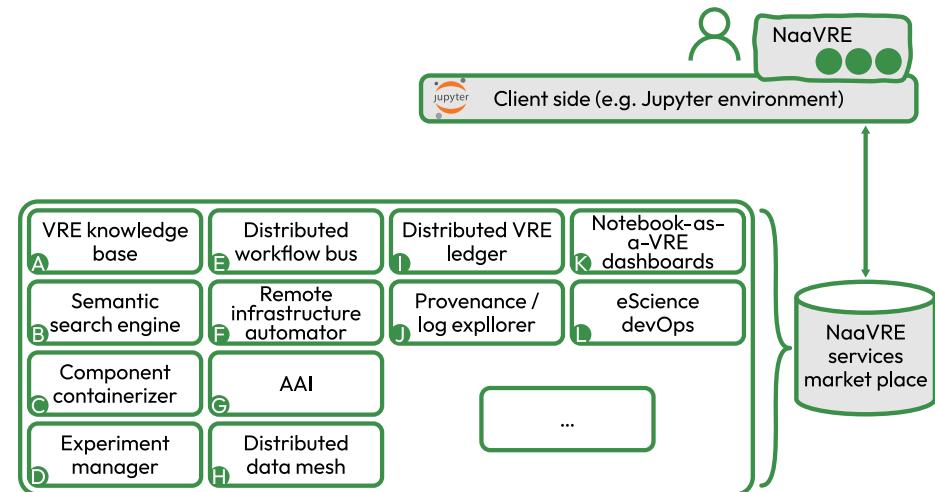
"Virtual Research Environments (VREs) provide user-centric support for discovering and selecting data and software services from different sources and composing and executing application workflows, ..." (Jeffery et al., 2020)

# How to support data-centric experiments

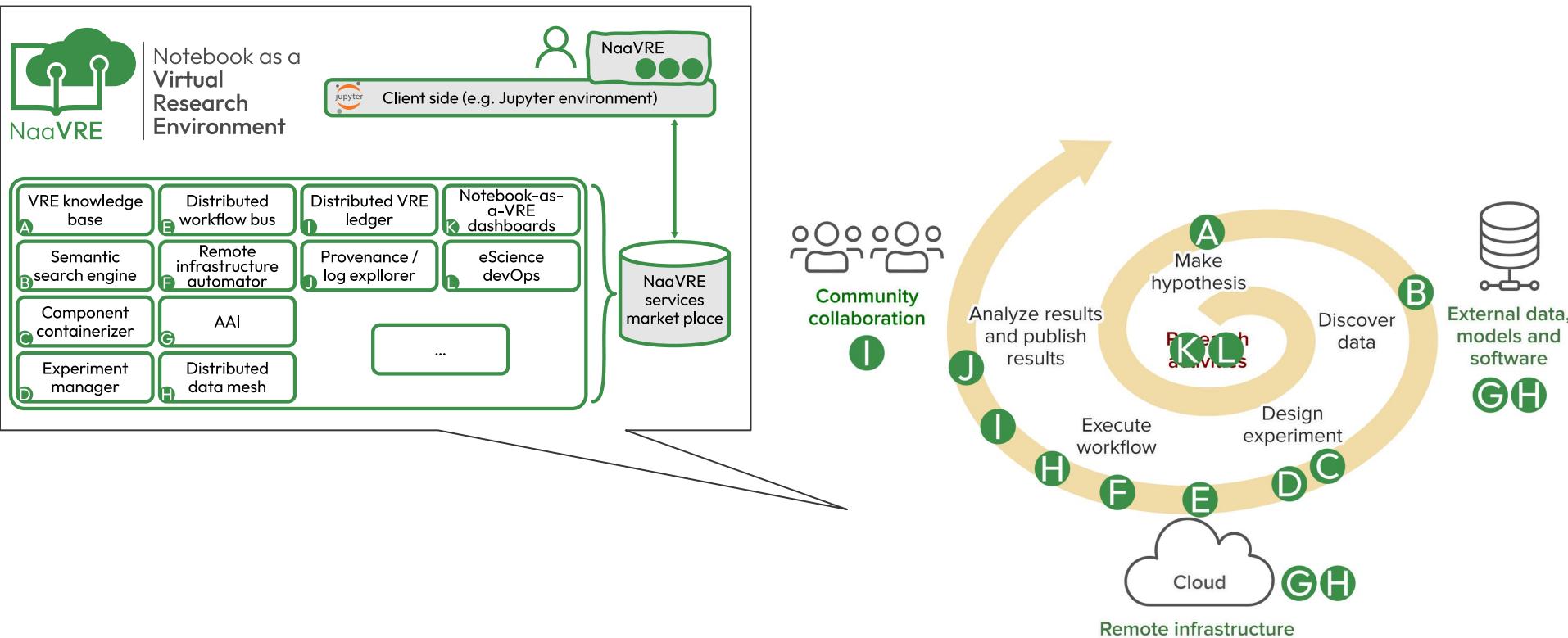
- **Computational notebooks**
  - Widely used by researchers
  - Documentation and visualization alongside code
  - Interactive code execution
  - → **developing and tweaking models**
- **Virtual research environment**
  - Collaboration
  - FAIR data, models and services
  - Remote infrastructure
  -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



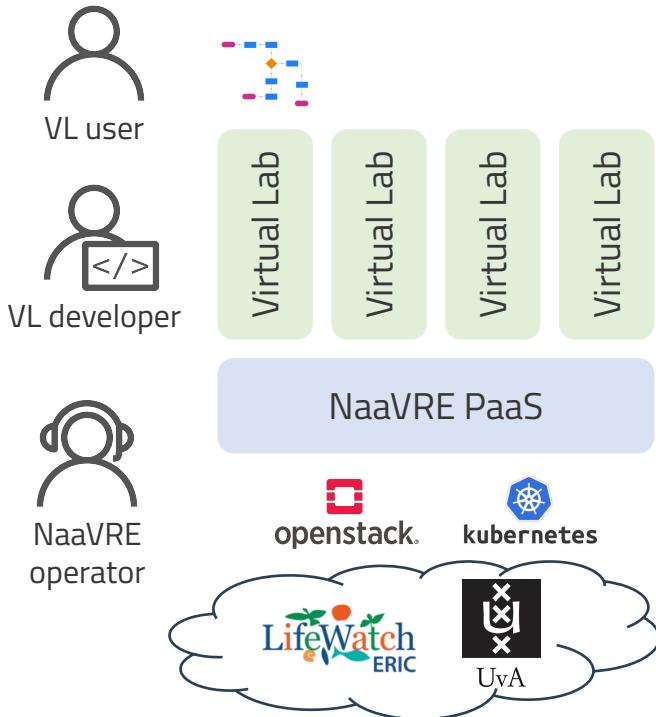
Notebook as a  
Virtual  
Research  
Environment



# Research activities and Jupyter extensions



# Notebook-as-a-VRE and Virtual Labs



The screenshot shows the [naavre.lifewatch.dev/vreapp](https://naavre.lifewatch.dev/vreapp) web interface:

- Header:** https://naavre.lifewatch.dev/vreapp
- Left sidebar:**
  - Home (selected)
  - About
  - Documentation
  - Login
- Section: NaaVRE virtual research environments**

A collection of virtual research environments powered by NaaVRE.

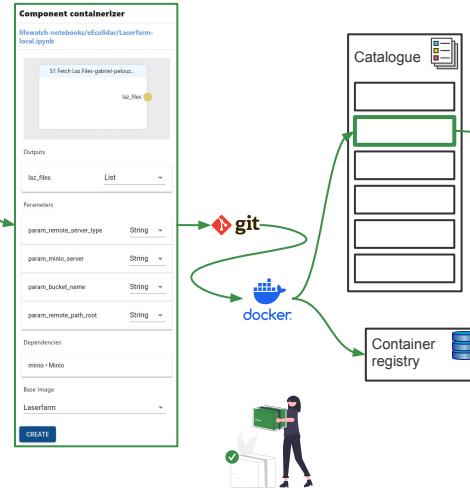
If you wish to help us improve NaaVRE, follow this short [tutorials](#) and fill in this [form](#).
- Grid of virtual labs:**

<b>NaaVRE Open Lab</b> Open experimentation with virtual labs	<b>Vol2bird collaborative virtual labs</b> Vertical profiling of biological scatterers	<b>Laserfarm collaborative virtual labs</b> LiDAR point cloud analysis for macro-ecology

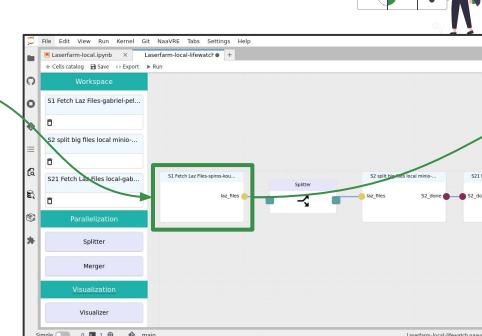
# From notebooks to cloud workflows

## 1. PROTOTYPE MODEL IN NOTEBOOK

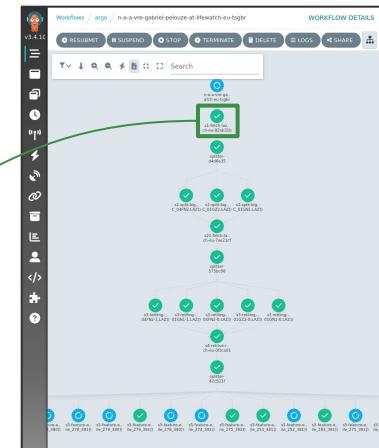
## 2. CONTAINERIZE CELLS



### 3. COMPOSE A WORKFLOW



## 4. RUN IT IN THE CLOUD



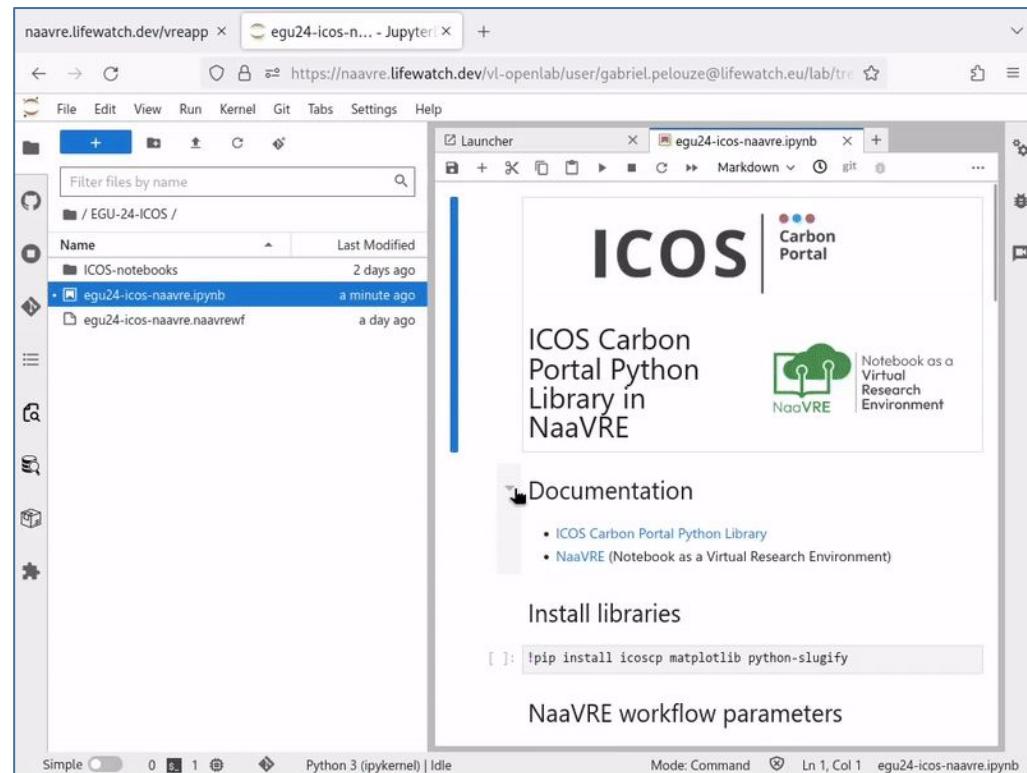
# From notebooks to cloud workflows

## 1. PROTOTYPE MODEL IN NOTEBOOK

## 2. CONTAINERIZE CELLS

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

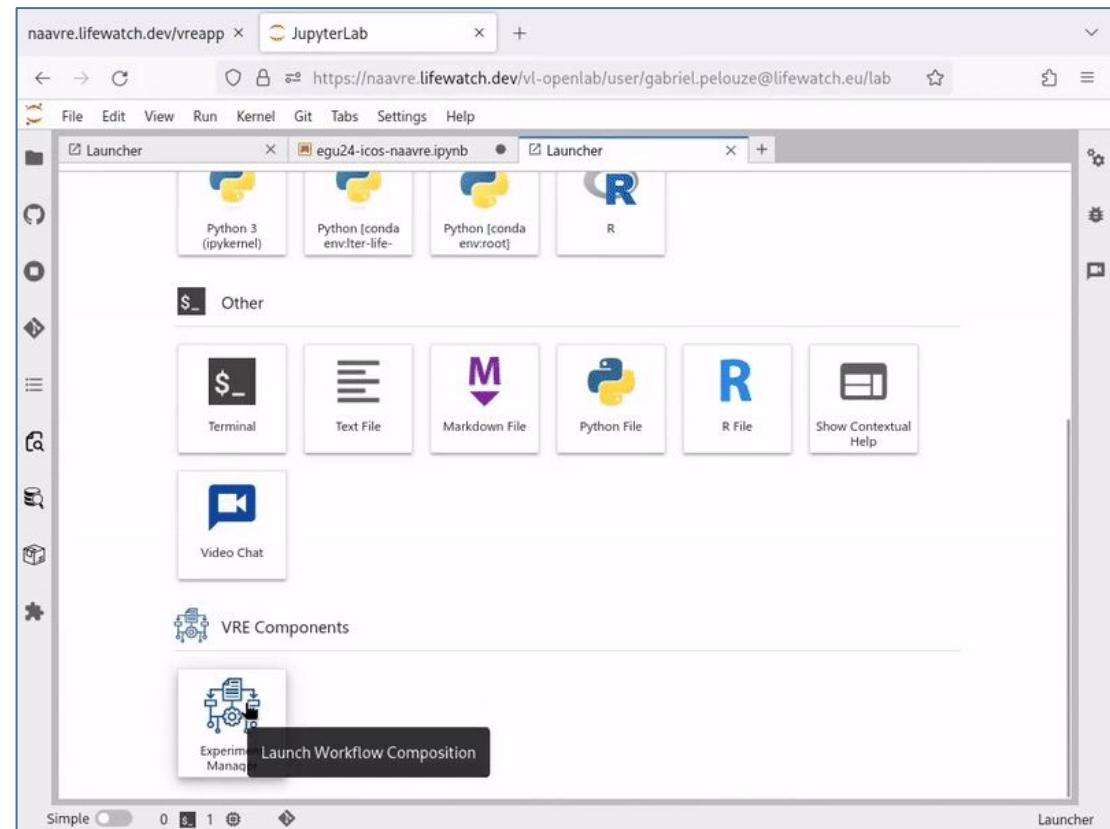
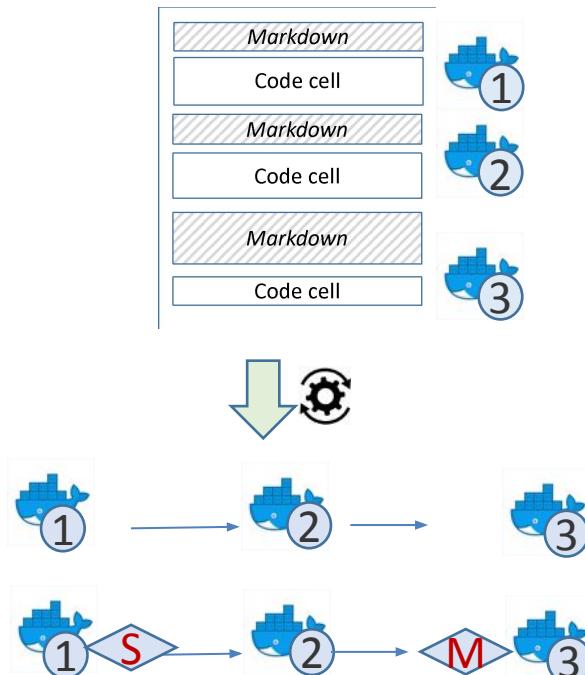
Code cell → 



# From notebooks to cloud workflows

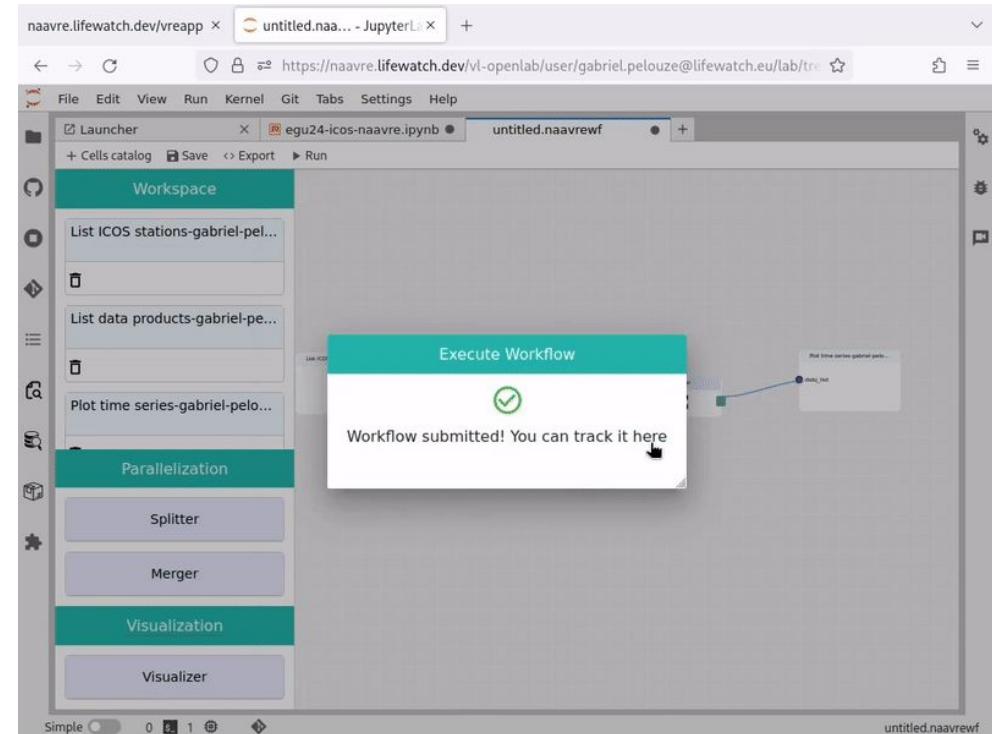
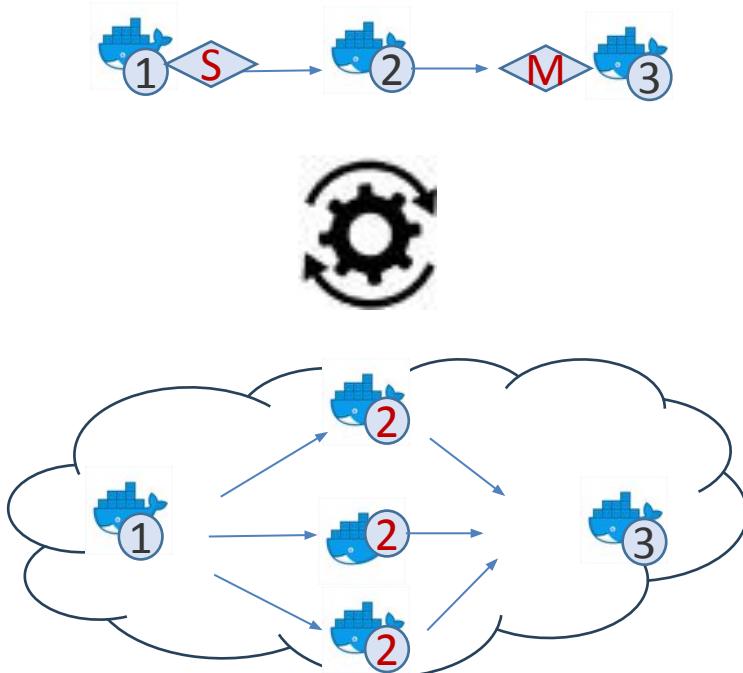
## 3. COMPOSE A WORKFLOW: Customize data flow and input

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

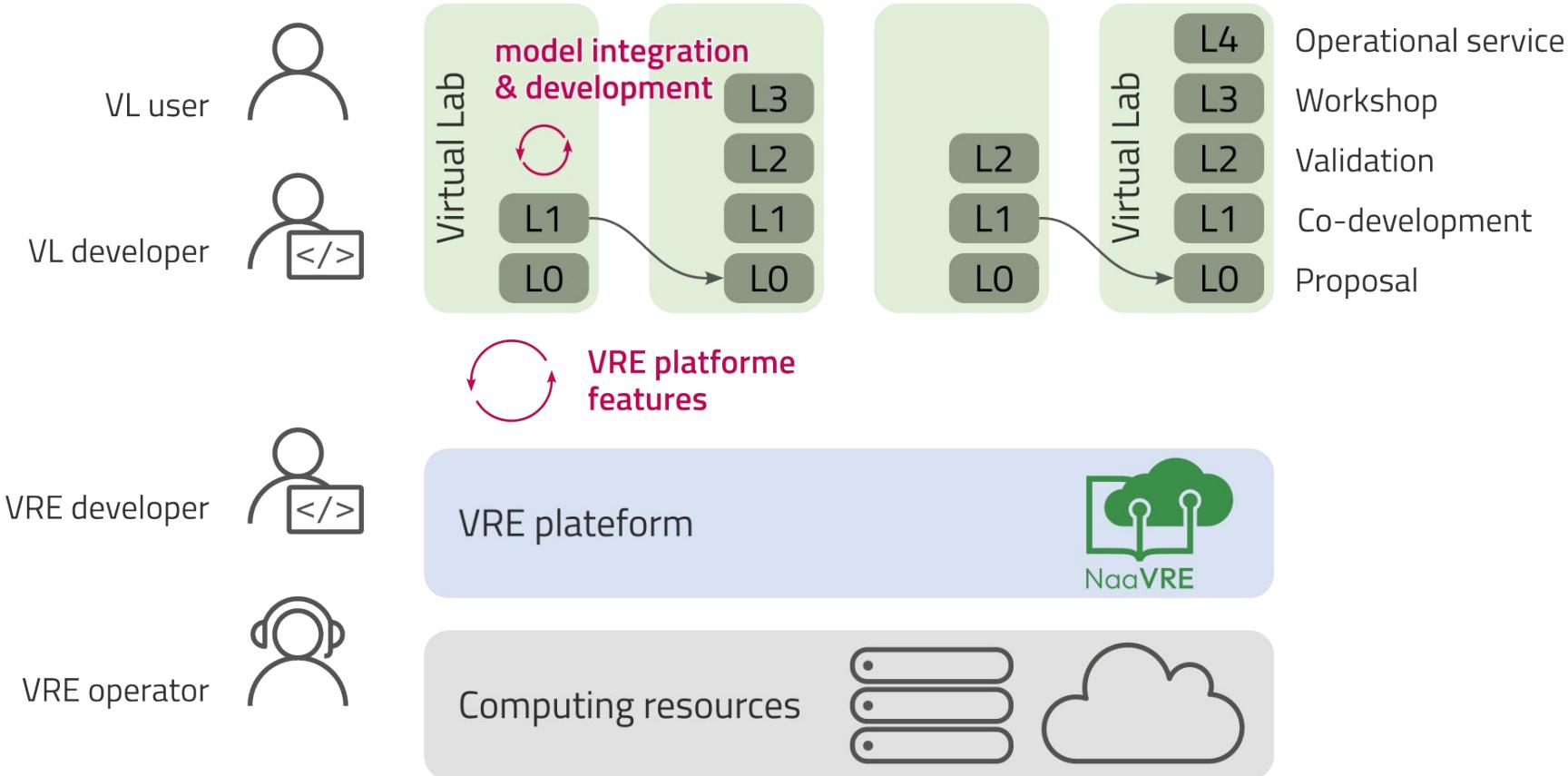


# From notebooks to cloud workflows

## 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>

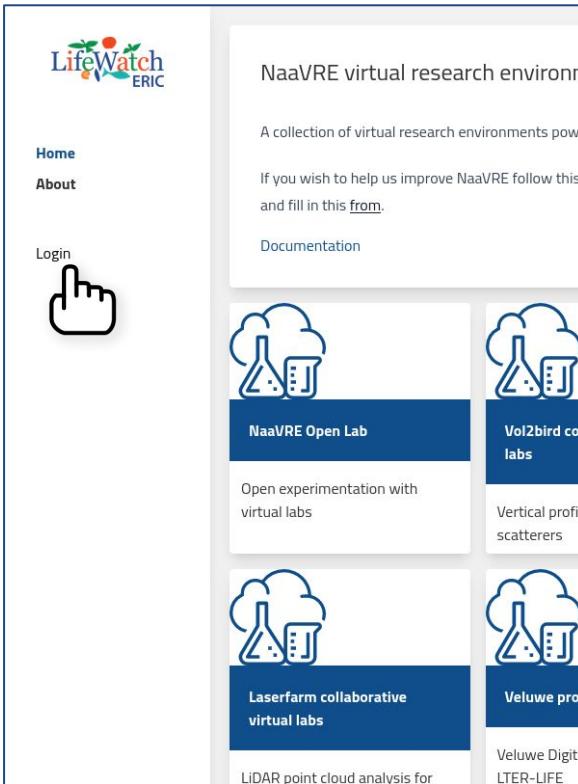


Screenshot of a web browser showing the NaaVRE PaaS demo page. The URL in the address bar is [new.demo.naavre.net/vreapp#](https://new.demo.naavre.net/vreapp#). The page features the LifeWatch ERIC logo and navigation links for Home, About, and Login. A prominent message reads: "The new NaaVRE. A collection of virtual labs powered by NaaVRE. 🚨 Warning! This is a preview version, which is subject to change without notice." Below this are two main sections: "NaaVRE Open Lab" (with an icon of a cloud and flasks) and "Laserfarm collaborative virtual labs" (with an icon of a plane and a tree). The footer of the page states: "Powered by NaaVRE / LifeWatch ERIC VLIC (About)".



Starting your virtual lab

# Sign in



NaaVRE virtual research environment

A collection of virtual research environments powered by the NaaVRE platform.

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

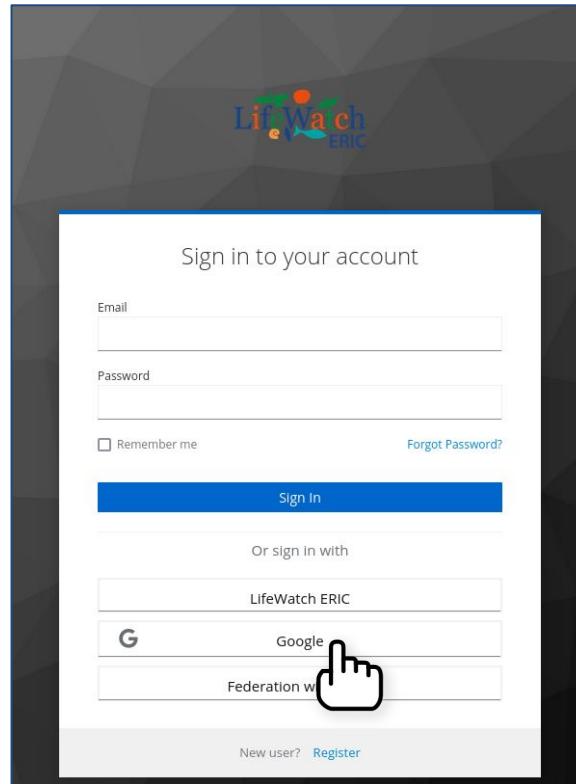
Documentation

**NaaVRE Open Lab**  
Open experimentation with virtual labs

**Vol2bird co-labs**  
Vertical profile scatterers

**Laserfarm collaborative virtual labs**  
LiDAR point cloud analysis for

**Veluwe pro**  
Veluwe Digital Ecosystem - LIFE



## Sign in to your account

Email

Password

Remember me [Forgot Password?](#)

**Sign In**

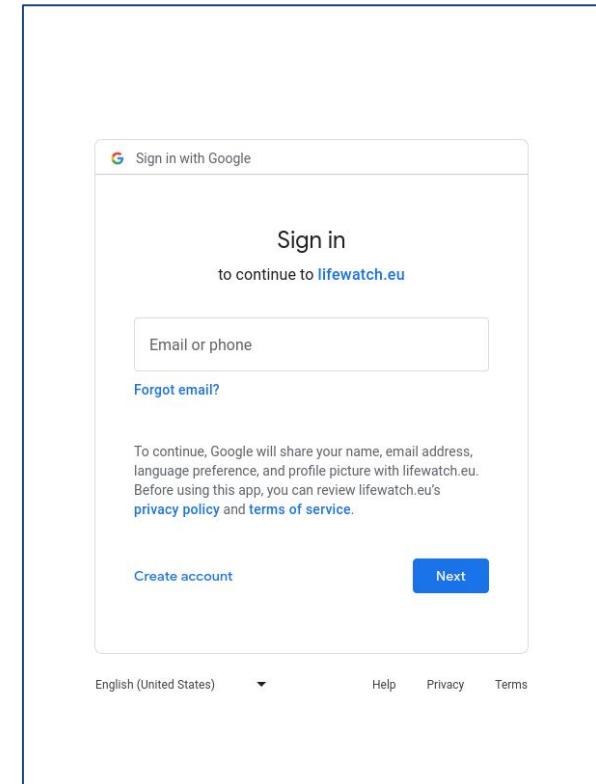
Or sign in with

LifeWatch ERIC

Google

Federation

New user? [Register](#)



Sign in with Google

## Sign in

to continue to [lifewatch.eu](#)

Email or phone

[Forgot email?](#)

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

English (United States) ▾ [Help](#) [Privacy](#) [Terms](#)



Starting your virtual lab

# Pick your collaborative virtual labs

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

 Laserfarm collaborative virtual labs

Open experiment virtual labs

Powered by NaaVRE / LifeWatch ERIC VLIC (About)

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



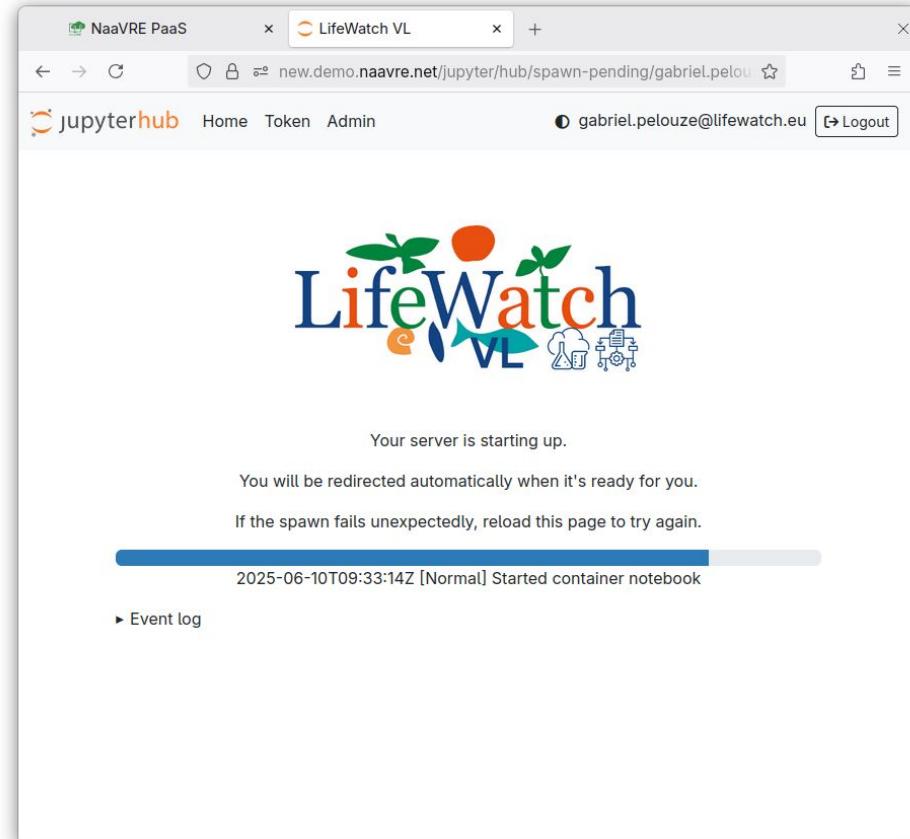
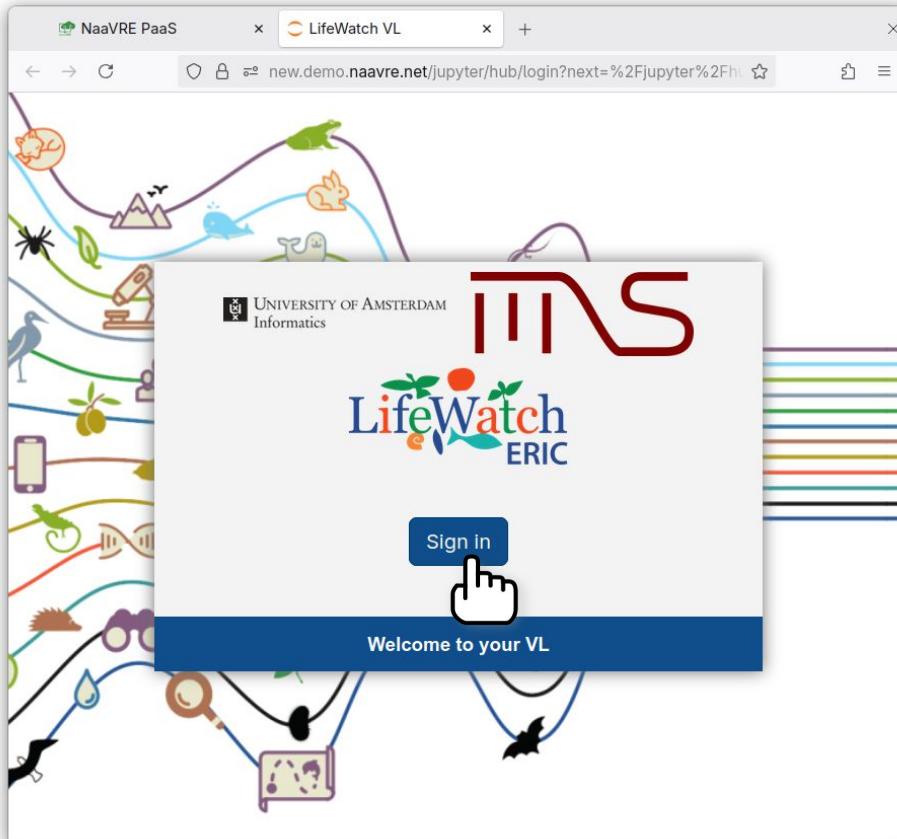
### Assets

Workflow runs Data Products Geographic data products

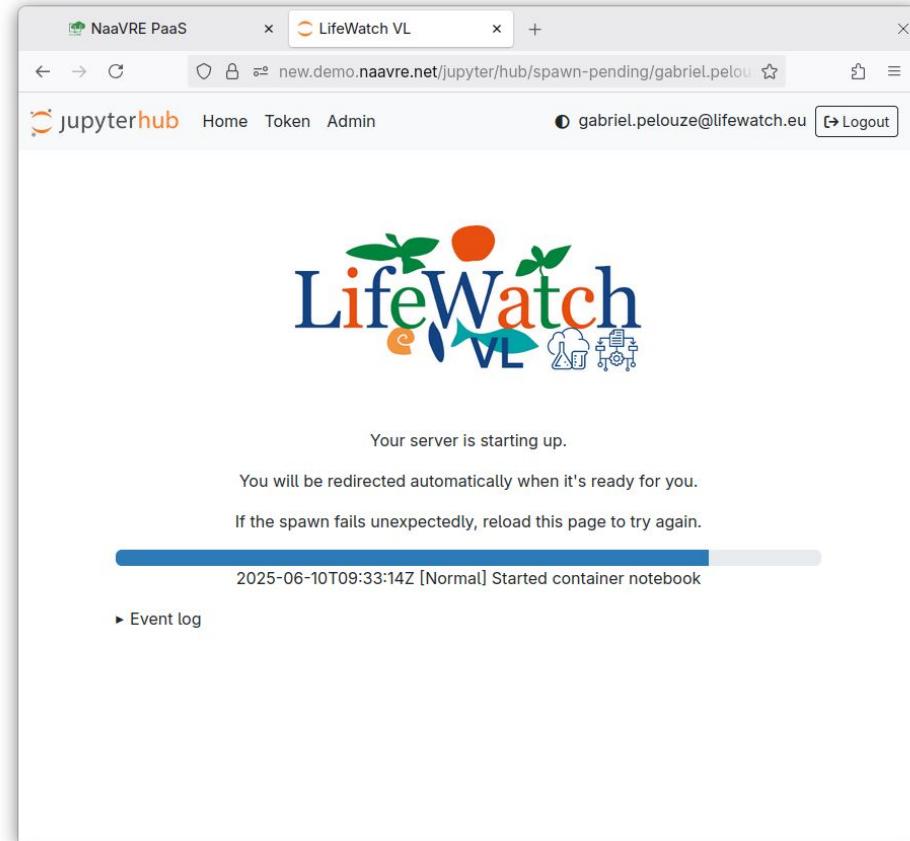
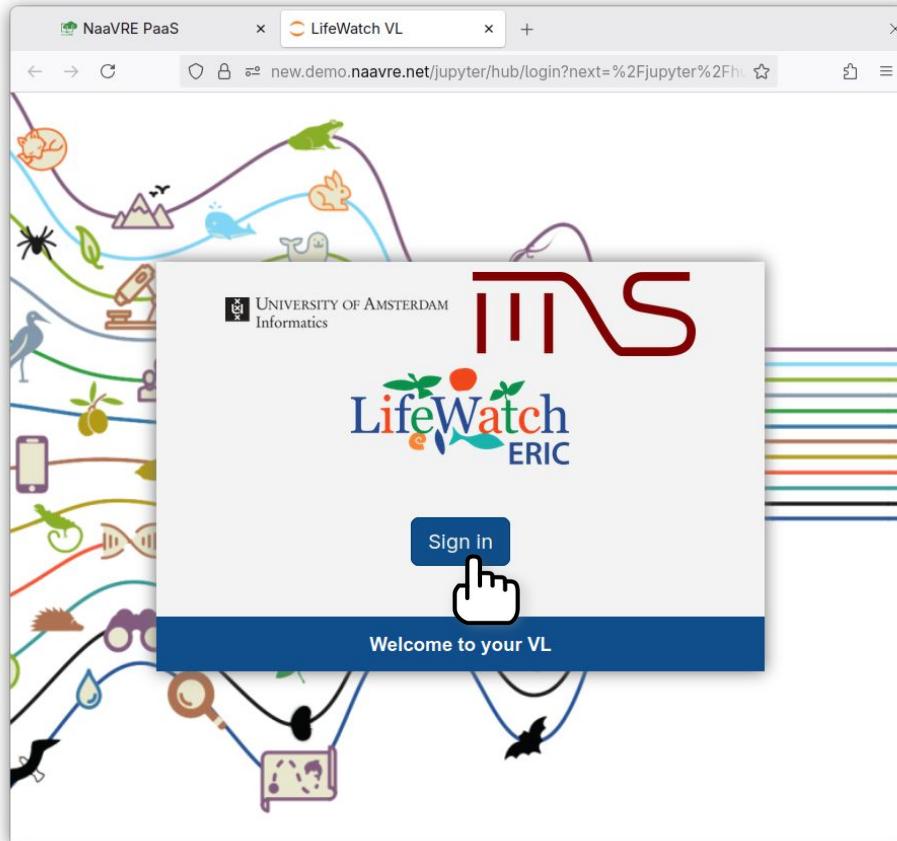


0 workflow runs

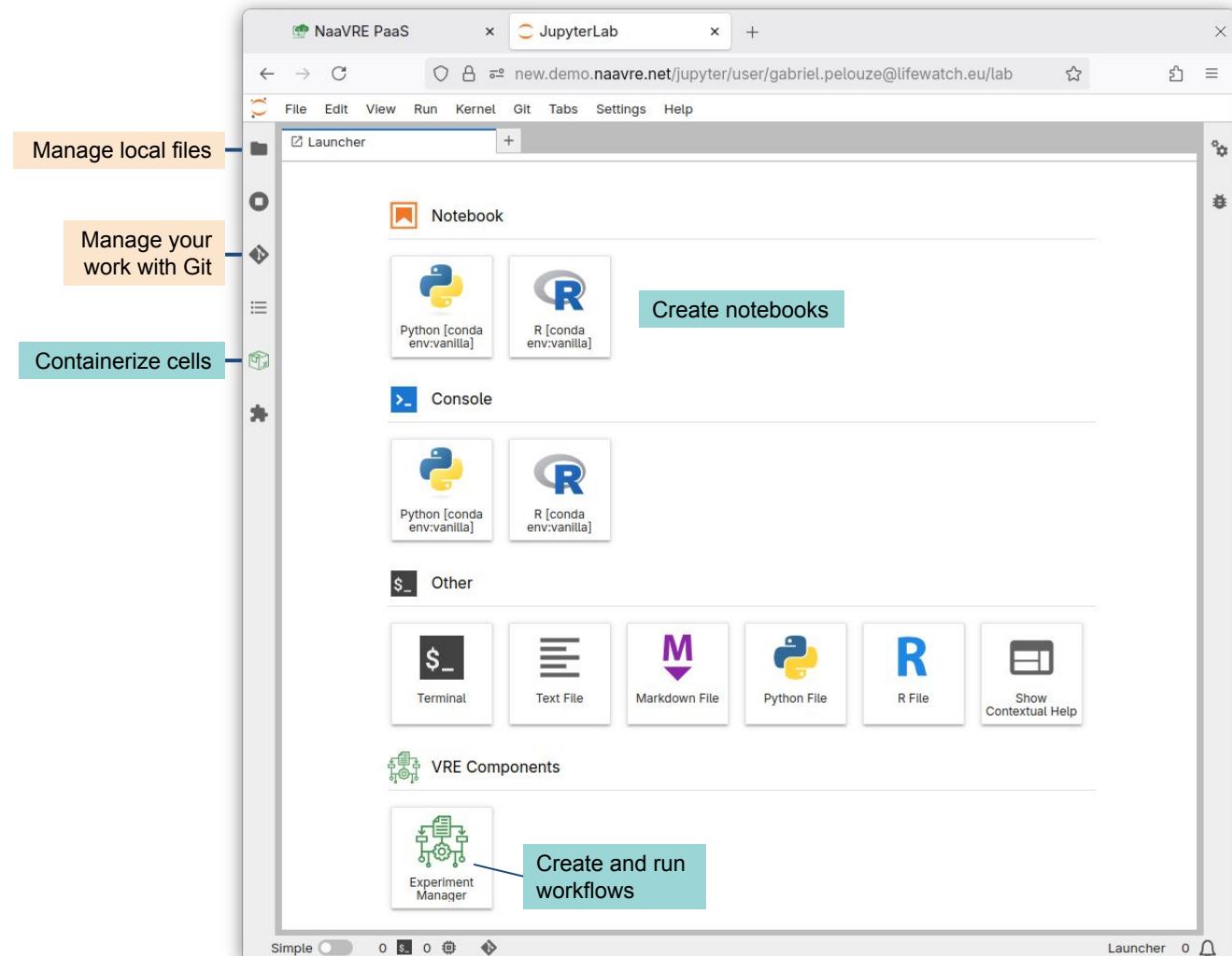
# Pick your collaborative virtual labs



# Start your virtual lab

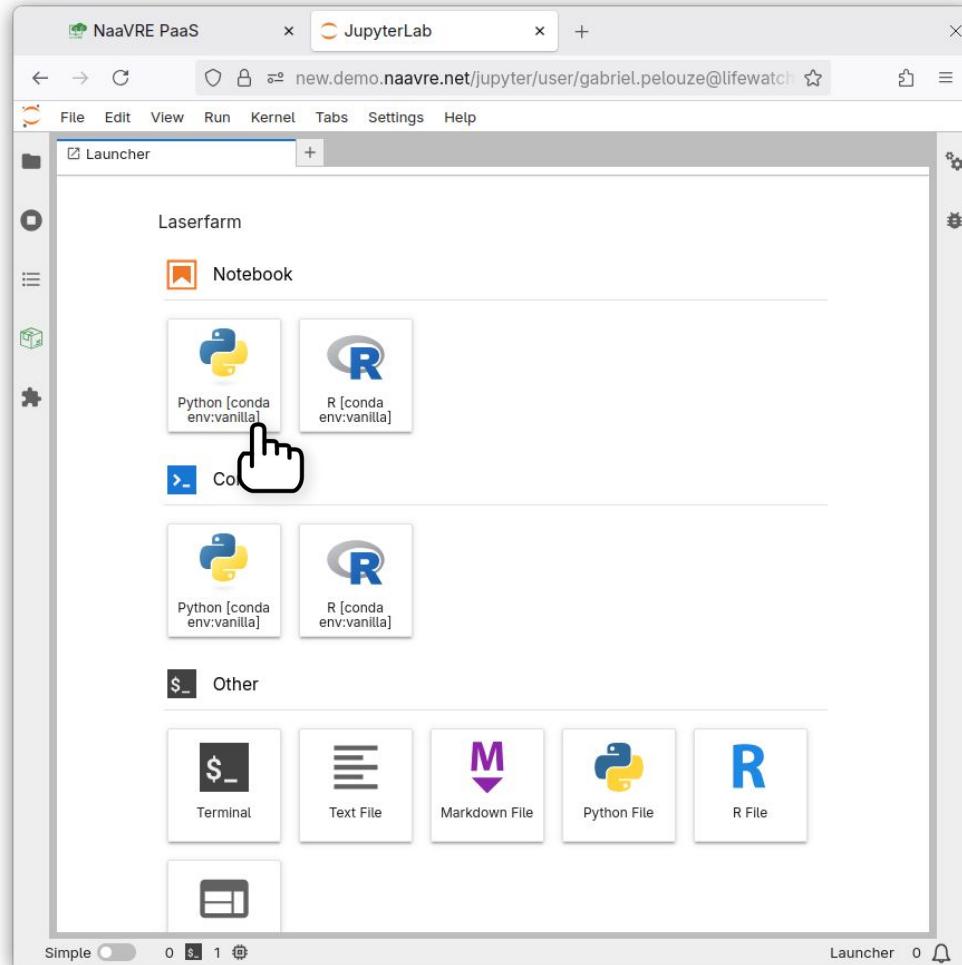


# The NaaVRE interface



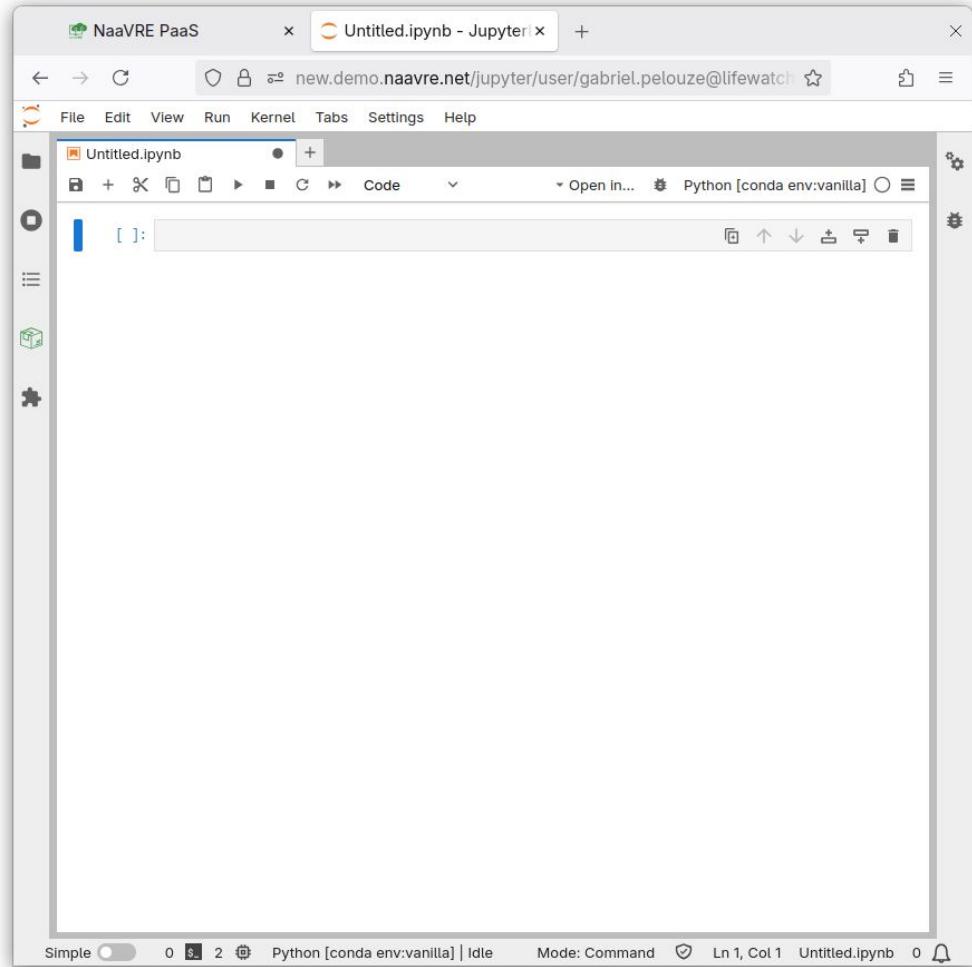
# Create a notebook

## 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

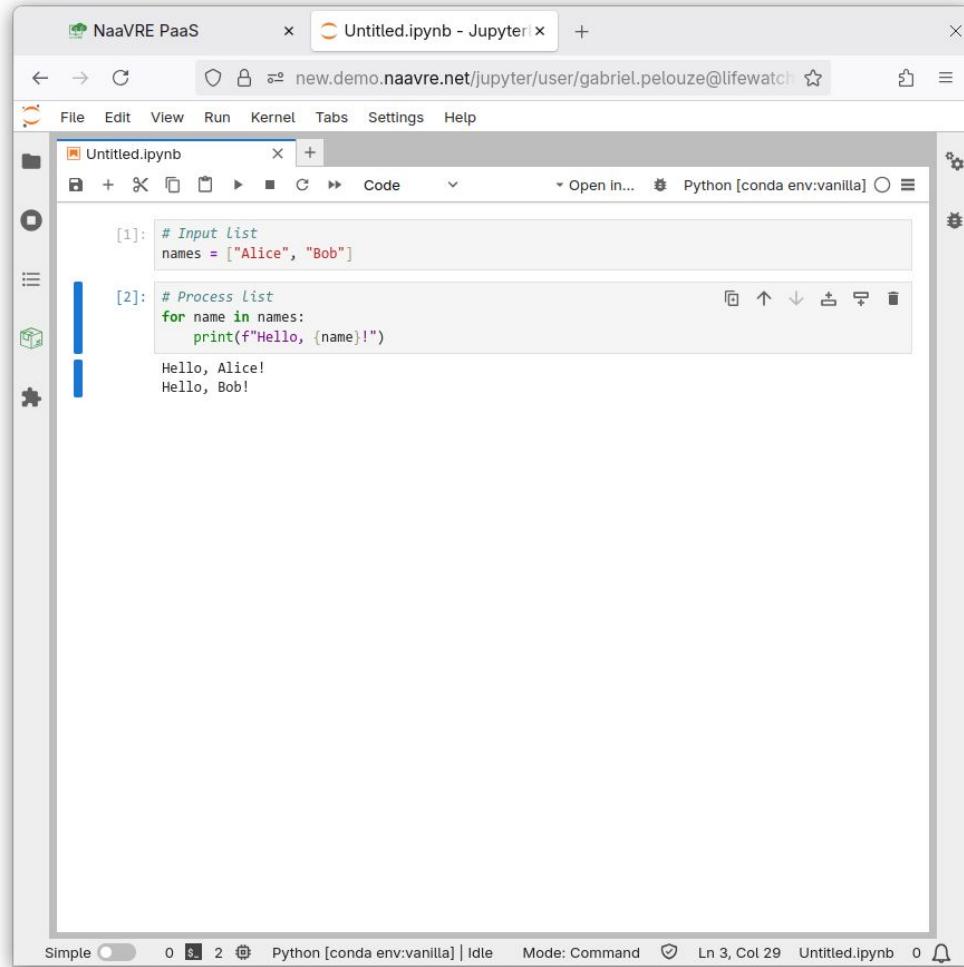
```
# Input List
names = ["Alice", "Bob"]
```

```
# 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))
}
```



The screenshot shows a Jupyter Notebook interface with the following content:

```
File Edit View Run Kernel Tabs Settings Help
Untitled.ipynb + 
+ X Open in... Python [conda env:vanilla] 
[1]: # Input List
names = ["Alice", "Bob"]

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

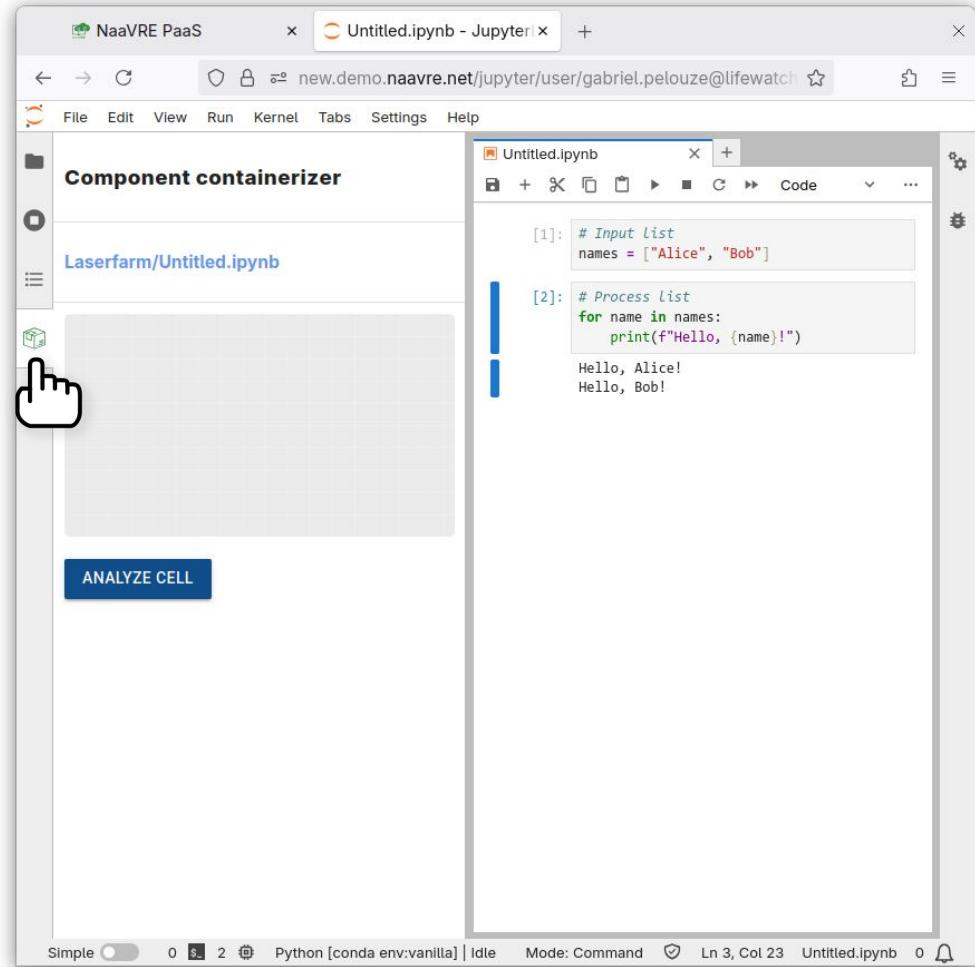
Hello, Alice!
Hello, Bob!
```

The interface includes a toolbar with File, Edit, View, Run, Kernel, Tabs, Settings, and Help. The notebook title is "Untitled.ipynb". The code cells are numbered [1] and [2]. The output of cell [2] shows the names "Alice" and "Bob" being printed with "Hello," in front of them. The bottom status bar shows "Simple" mode, 0 cells run, Python [conda env:vanilla] | Idle, Mode: Command, Ln 3, Col 29, Untitled.ipynb, and a bell icon.



# Create a notebook

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



The screenshot shows a Jupyter Notebook interface with the following details:

- Header:** NaaVRE PaaS, Untitled.ipynb - Jupyter
- Toolbar:** File, Edit, View, Run, Kernel, Tabs, Settings, Help
- Left Sidebar:** Component containerizer, Laserfarm/Untitled.ipynb
- Code Cell 1:** [1]: 

```
# Input list
names = ["Alice", "Bob"]
```
- Code Cell 2:** [2]: 

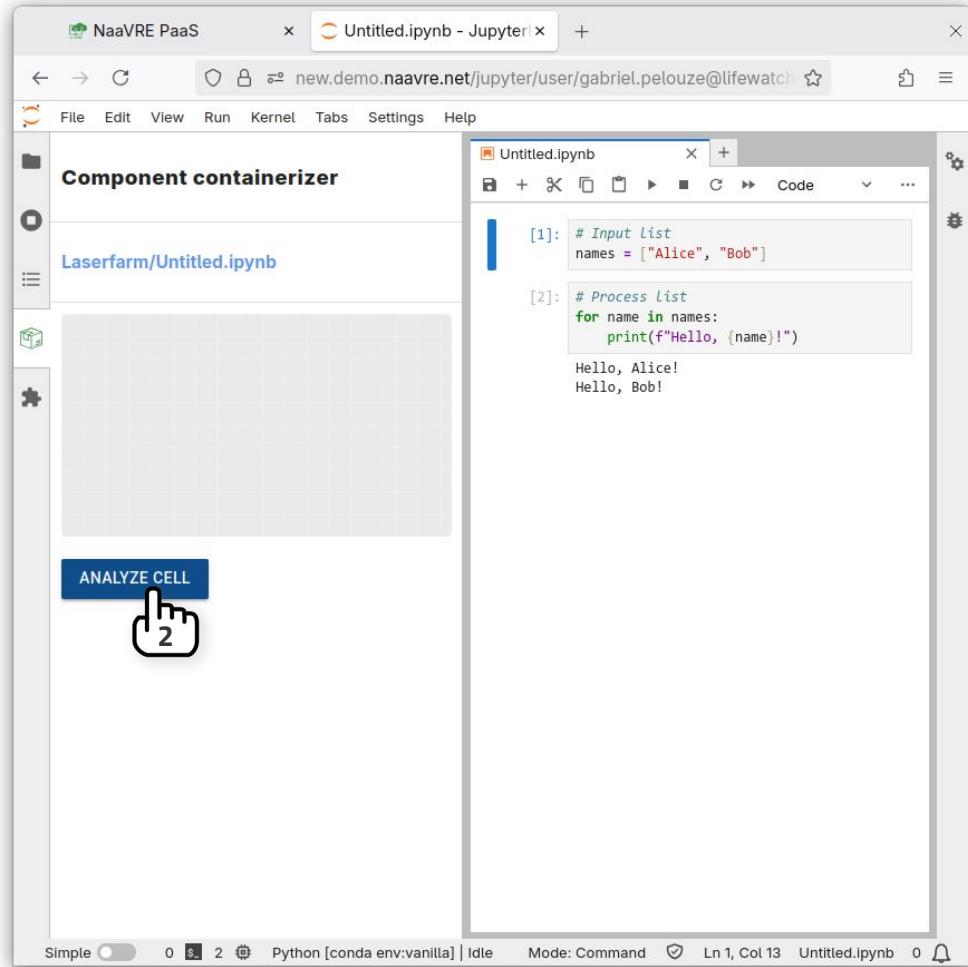
```
# Process List
for name in names:
    print(f"Hello, {name}!")
```

Output: Hello, Alice!  
Hello, Bob!
- Bottom Status Bar:** Simple, 0, Python [conda env:vanilla] | Idle, Mode: Command, Ln 3, Col 23, Untitled.ipynb, 0, Bell icon



# 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"



The screenshot shows a Jupyter Notebook interface with the 'Component containerizer' extension. The top bar shows the title 'Untitled.ipynb - Jupyter' and the URL 'new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch'. The menu bar includes File, Edit, View, Run, Kernel, Tabs, Settings, and Help. The left sidebar shows a tree structure with 'Component containerizer' and 'Laserfarm/Untitled.ipynb'. The main area displays a code cell with the following Python code:

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

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

Hello, Alice!
Hello, Bob!
```

Below the code cell is a button labeled 'ANALYZE CELL' with a hand cursor icon pointing at it. The status bar at the bottom shows 'Simple' mode, 0 cells run, Python [conda env:vanilla] | Idle, Mode: Command, Ln 1, Col 13, Untitled.ipynb, and a bell icon.

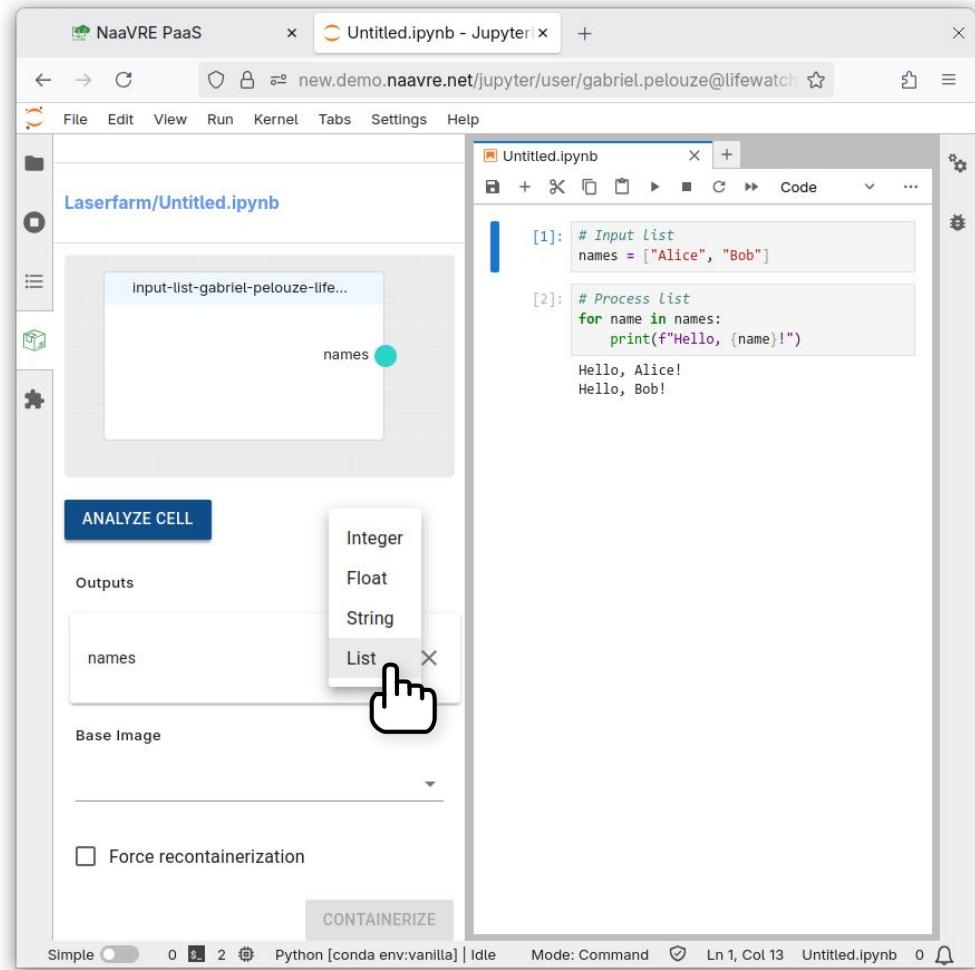


# Create a notebook

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

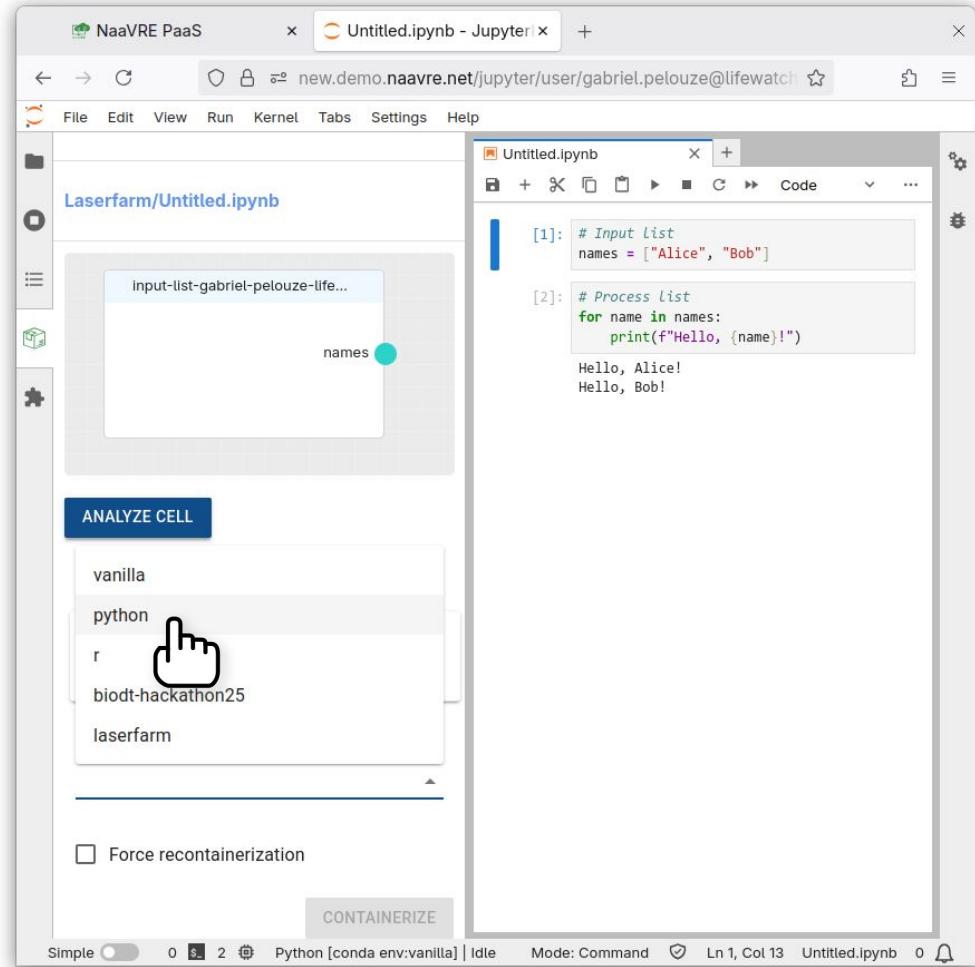
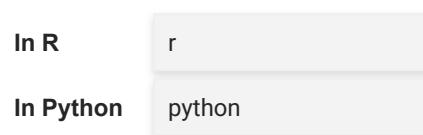
In R      List

In Python      List (set automatically)



# 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



Your first workflow

# 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 shows the NaaVRE PaaS interface. At the top, there are two tabs: "NaaVRE PaaS" and "Untitled.ipynb - Jupyter". The URL in the address bar is "new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch". The main window displays a Jupyter notebook titled "Untitled.ipynb" with the following code:

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

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

Hello, Alice!
Hello, Bob!
```

Below the notebook, a component containerizer dialog is open for the first cell. It shows the cell content and the variable "names" highlighted with a teal circle. The dialog has the following sections:

- ANALYZE CELL** button
- Outputs** section: "names" with a dropdown menu set to "List".
- Base Image** section: "python" selected.
- Force recontainerization** checkbox (unchecked).
- CONTAINERIZE** button at the bottom, with a large black cursor arrow pointing to it.

The status bar at the bottom shows "Simple" mode, 0 \$, 2 Python [conda env:val], Mode: Command, and Ln 1, Col 13.



# 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 shows the NaaVRE PaaS interface. On the left, a sidebar displays a tree structure for 'Laserfarm/Untitled.ipynb'. A cell in the notebook is selected, showing the code:[1]: # Input list
names = ["Alice", "Bob"]

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

Hello, Alice!
Hello, Bob!

Below the code, there is an 'ANALYZE CELL' button. On the right, a 'CONTAINERIZE' panel is open, showing the following configuration:

- Outputs: names (List)
- Base Image: python
- Force recontainerization

At the bottom right of the panel, there is a 'CONTAINERIZE' button. A success message is visible in the bottom right corner:

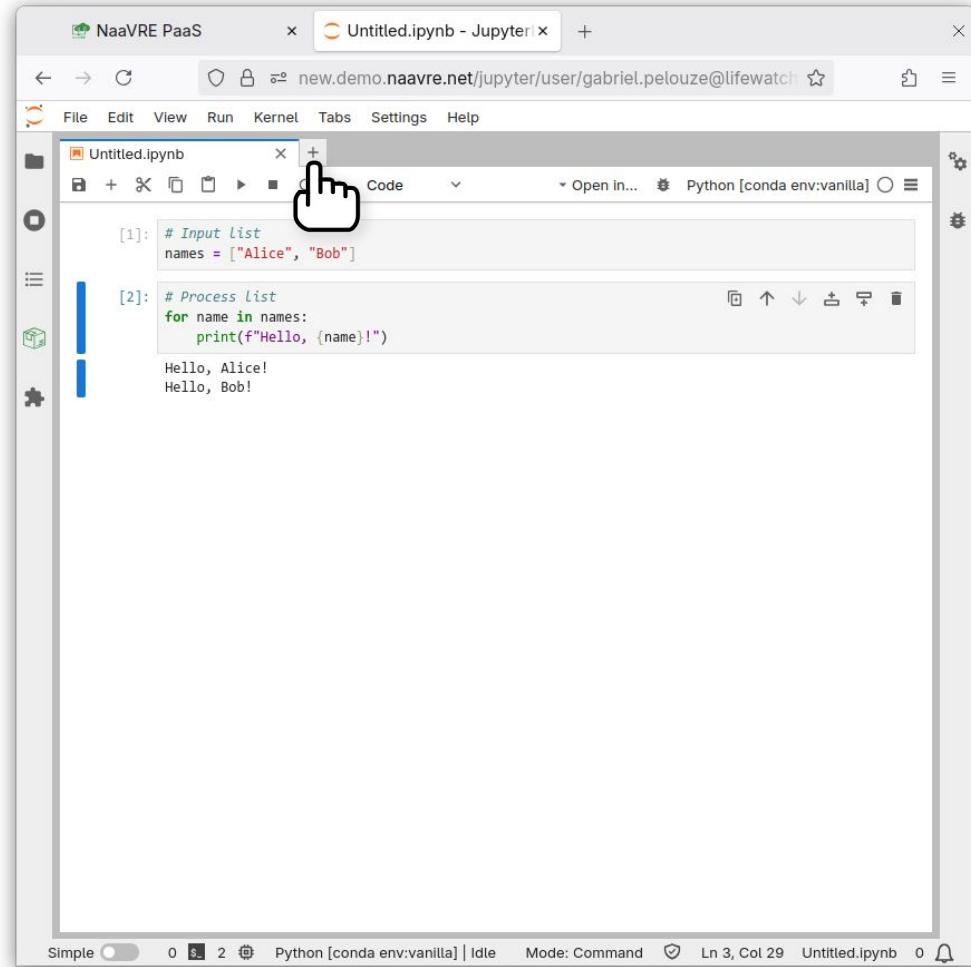
Added cell input-list-gabriel-pelouze-lifewatch-eu to the catalogue

Created cell input-list-gabriel-pelouze-lifewatch-eu



# Create a workflow

## 1. Open the experiment manager



The screenshot shows a Jupyter Notebook interface within a browser window titled "Untitled.ipynb - Jupyter". The browser URL is "new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch". The notebook has two cells:

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

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

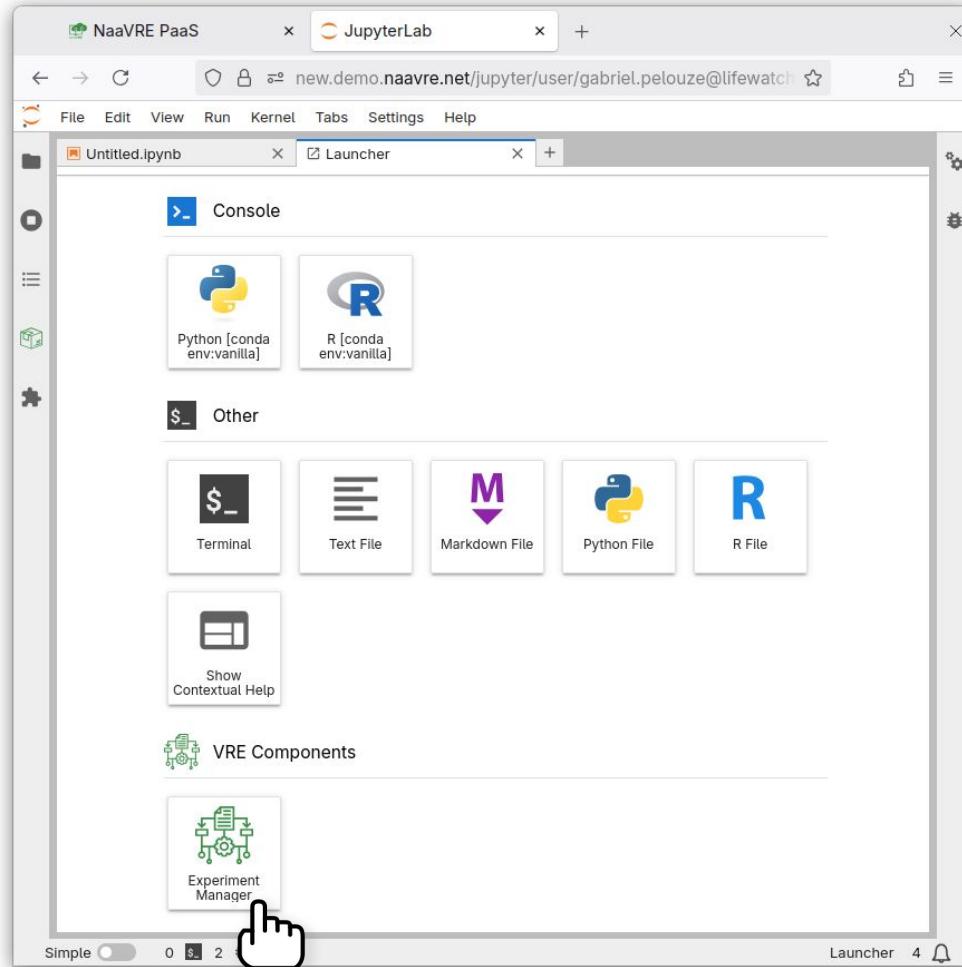
Hello, Alice!
Hello, Bob!
```

The '+' button in the toolbar is highlighted with a black circle and a hand cursor, indicating it can be used to add a new cell.



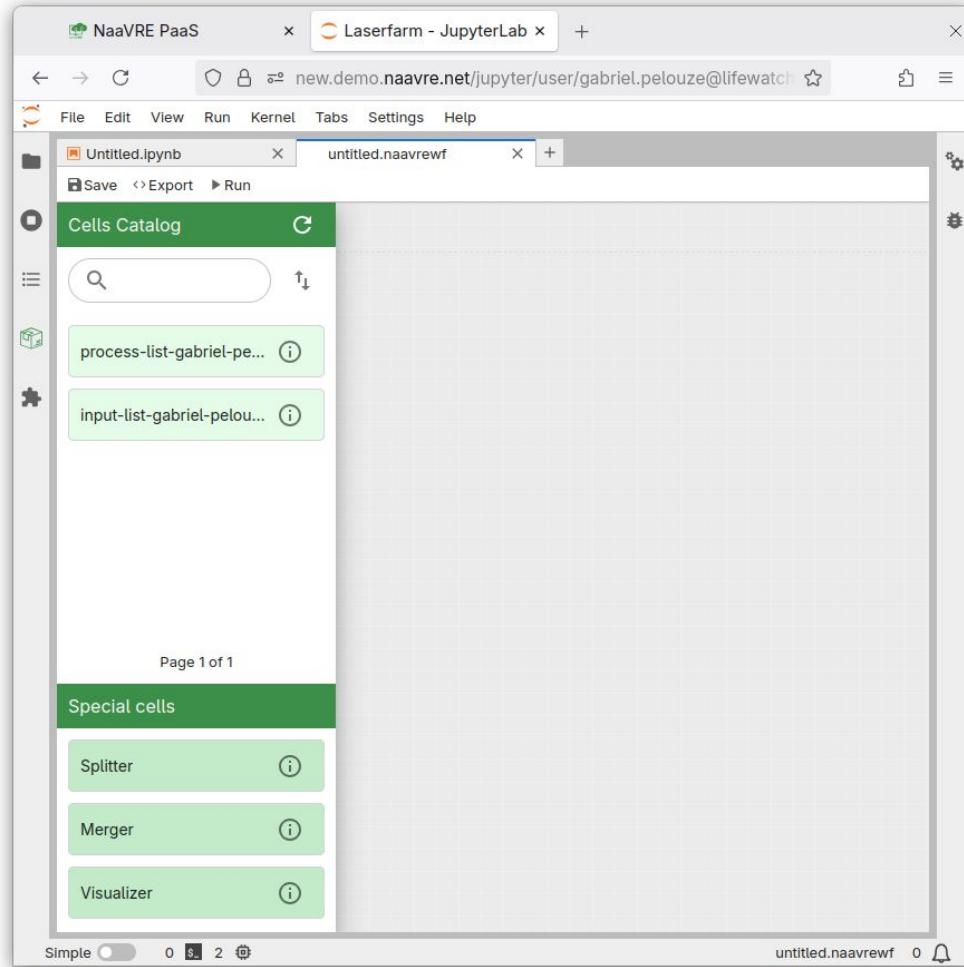
# Create a workflow

1. Open the experiment manager



# Create a workflow

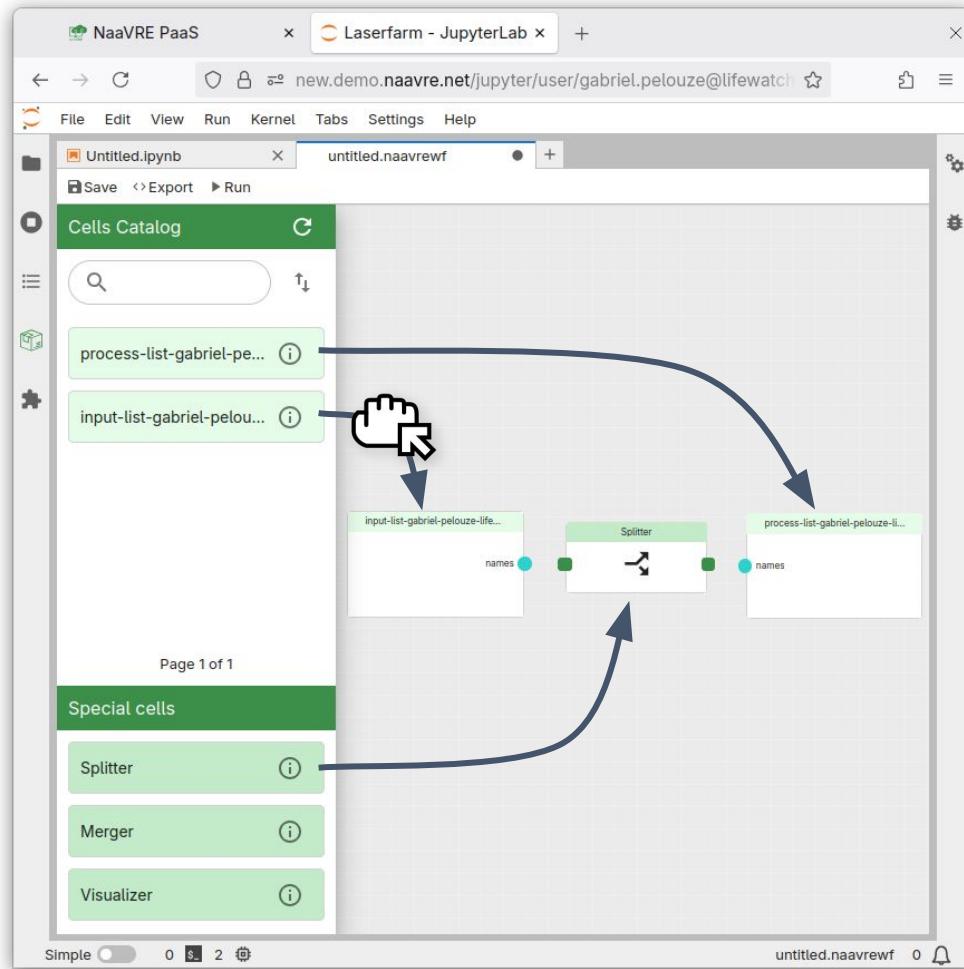
## 1. Open the experiment manager



Your first workflow

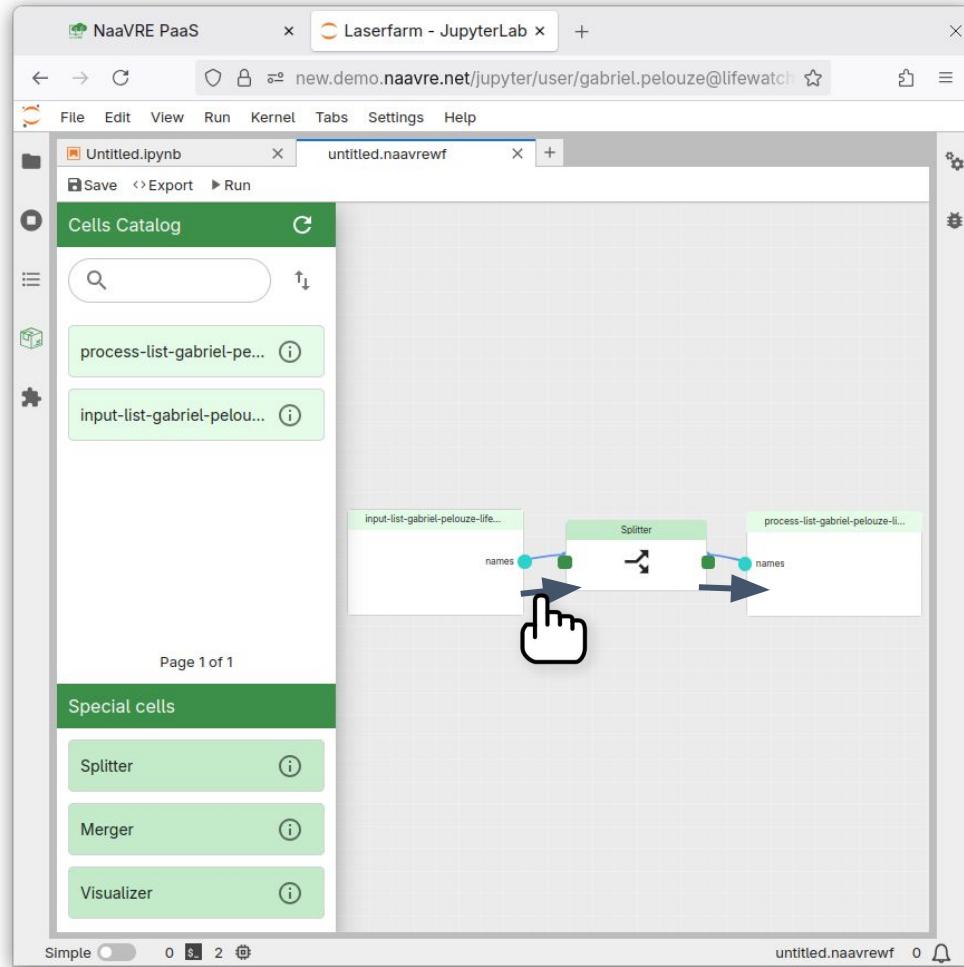
# Create a workflow

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



# Create a workflow

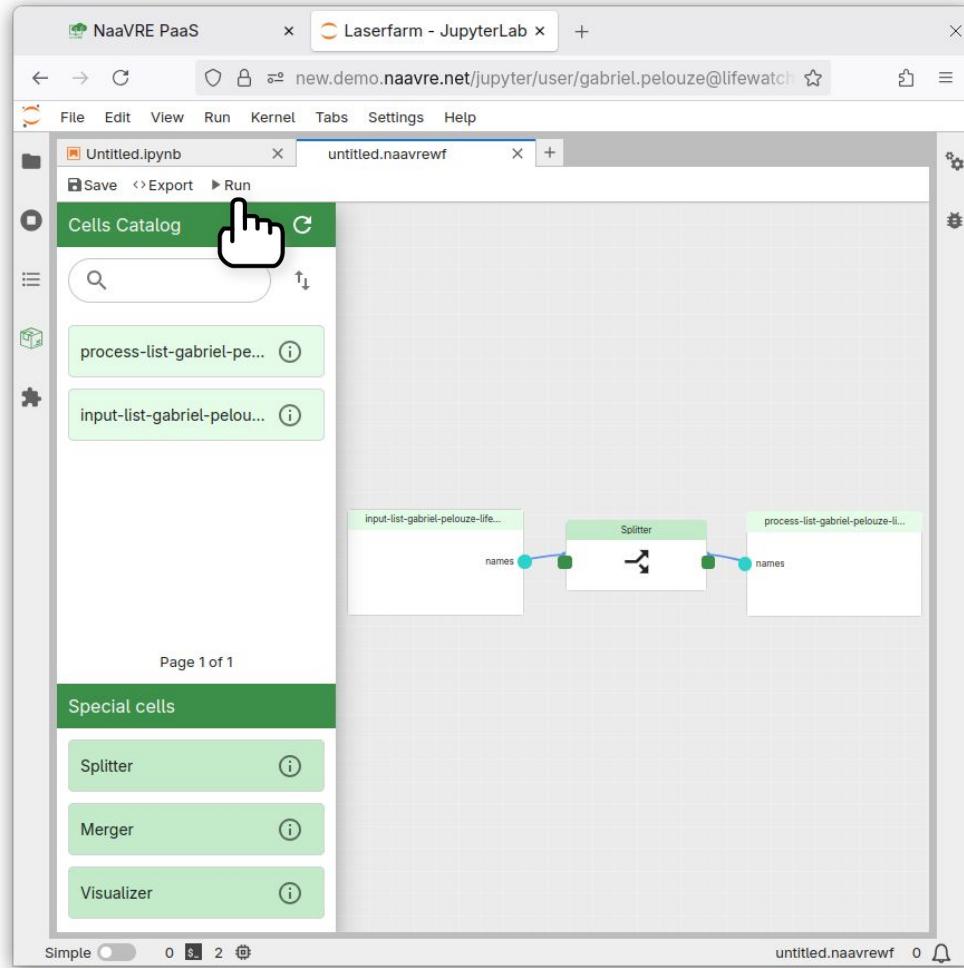
1. Open the experiment manager
2. Drag and drop the cells onto the canvas
3. Connect the cells



Your first workflow

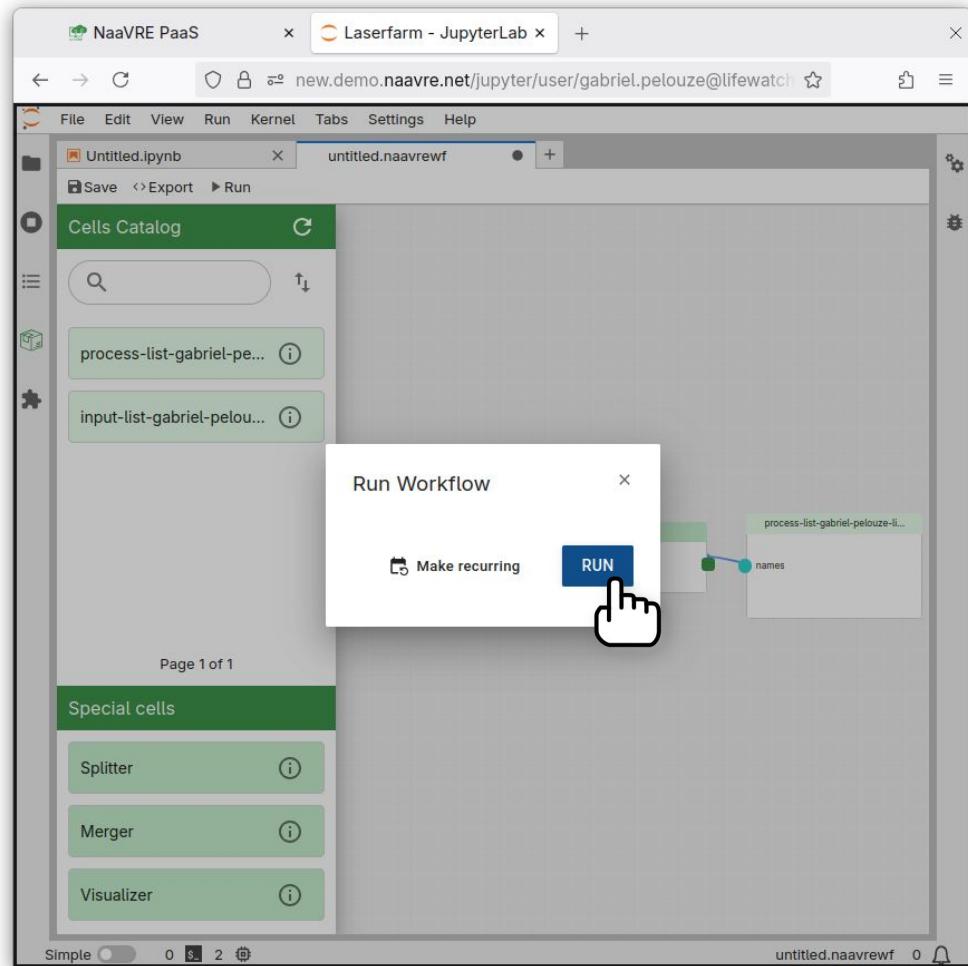
# Create a workflow

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



# Create a workflow

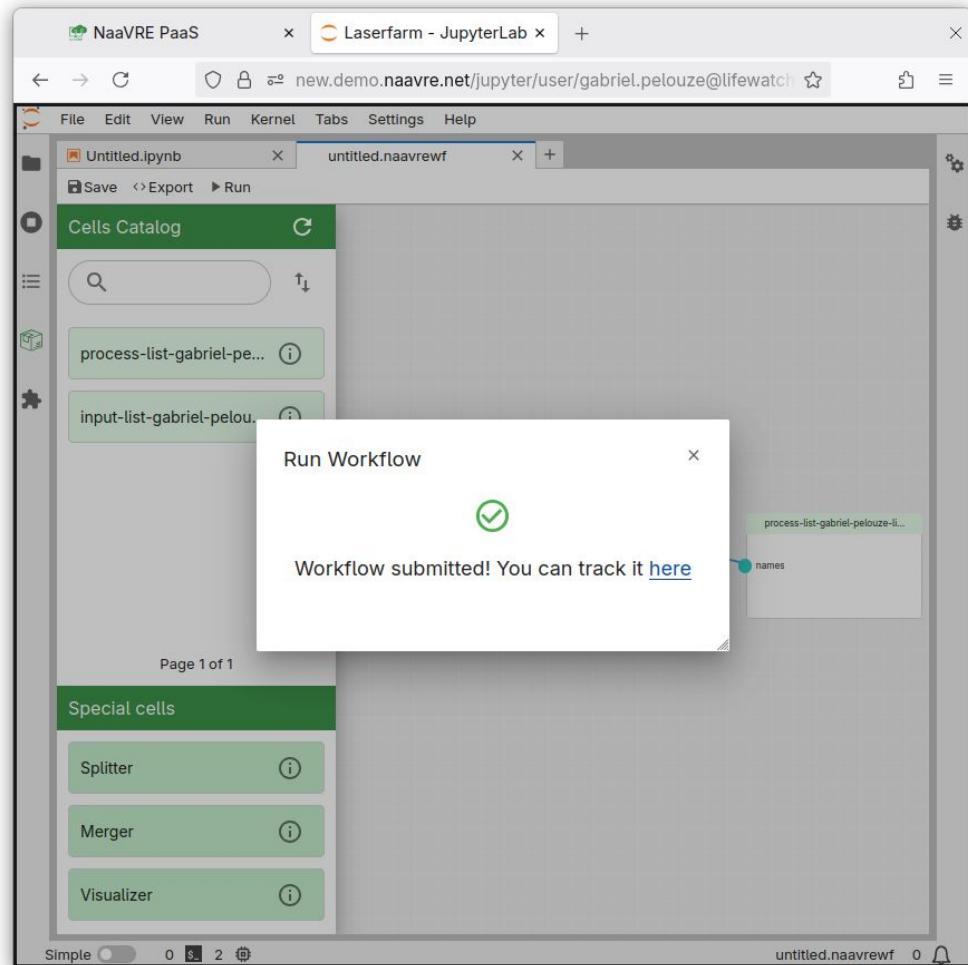
1. Open the experiment manager
2. Drag and drop the cells onto the canvas
3. Connect the cells
4. Execute the workflow



Your first workflow

# Create a workflow

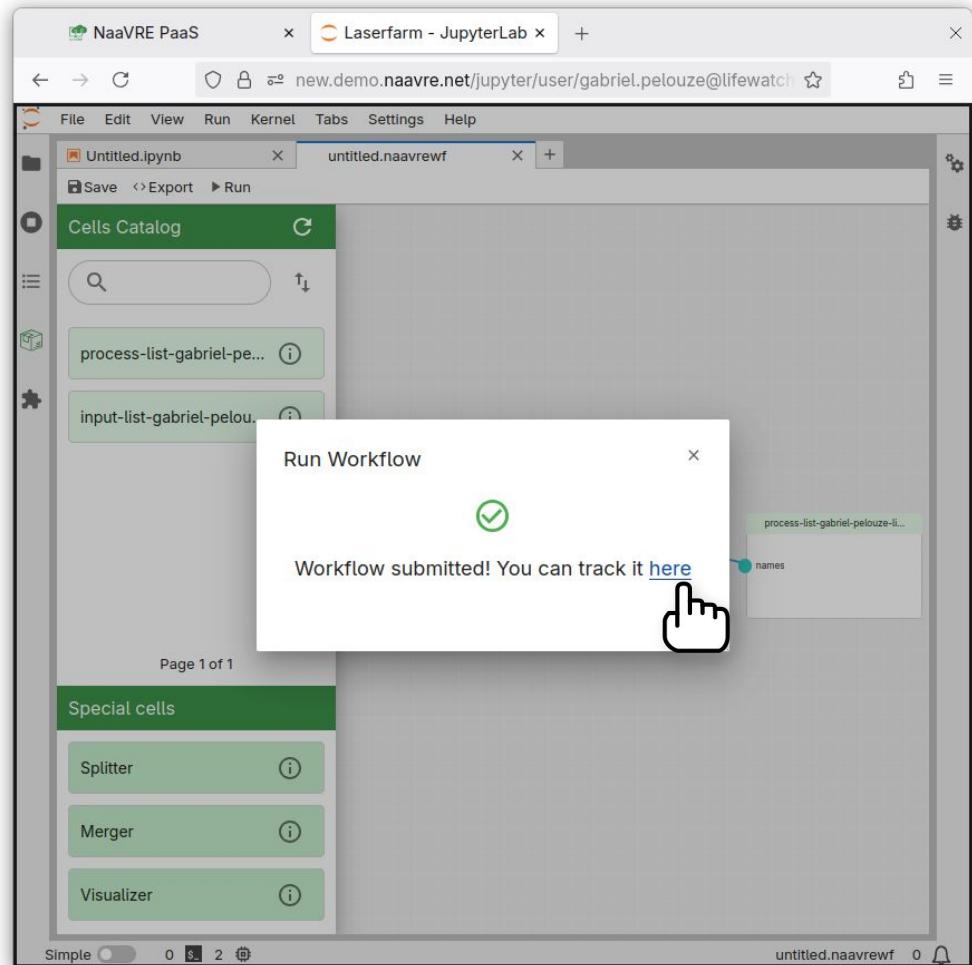
1. Open the experiment manager
2. Drag and drop the cells onto the canvas
3. Connect the cells
4. Execute the workflow
5. Well done!



Your first workflow

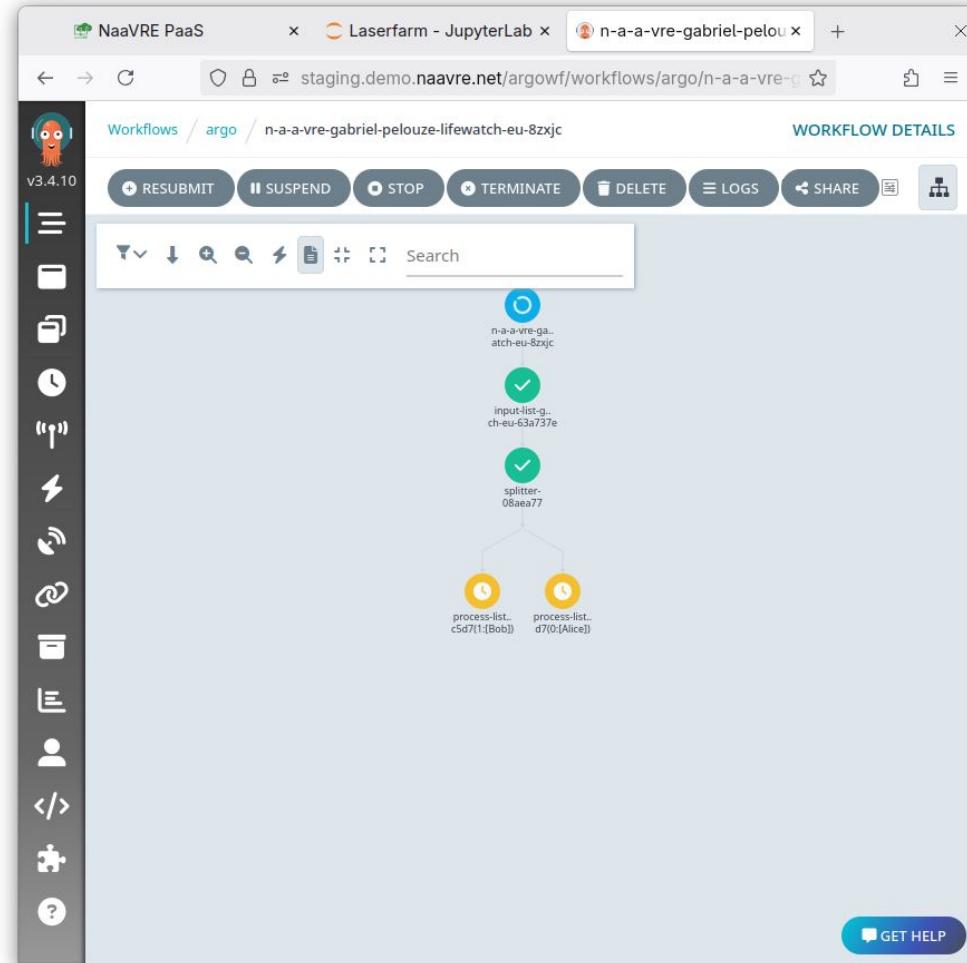
# Monitor a workflow

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



Your first workflow

# 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

NaaVRE PaaS x Exercise 2 s... - Jupyter +

new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch.eu/lab/tree/Open Lab/Git public/exercises/

File Edit View Run Kernel Git Tabs Settings Help

Exercise 2 split and merge x +

Exercise 2: Splitter and merger

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.

`# 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}!")`

Simple 1 2 main Python [conda env:vanilla] | Idle Mode: Command Ln 1, Col 1 Exercise 2 split and merge.ipynb 0

NaaVRE PaaS x Solution 2.n... - Jupyter +

new.demo.naavre.net/jupyter/user/gabriel.pelouze@lifewatch.eu/lab/tree/Open Lab/Git public/exercises/

File Edit View Run Kernel Git Tabs Settings Help

Exercise 2 split and merge x Solution 2.naavrewf +

Save Export Run

Cells Catalog

untitled-gabriel-pelouze...  
ex3-1-create-file-gabri...  
ex3-3-upload-file-gabri...  
ex3-2-plot-file-gabriel...  
ex2-3-print-list-gabriel...  
ex2-1-input-list-gabriel...  
ex2-2-process-list-gab...

ex2-1-input-list-gpelouze

names

Splitter

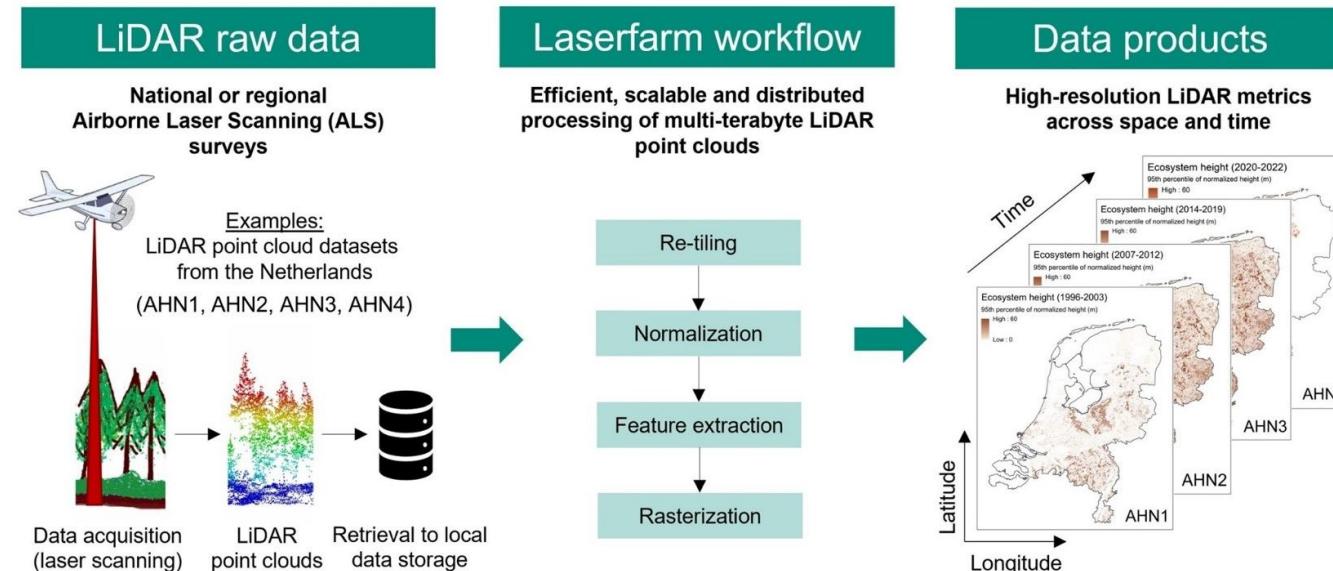
Simple 1 2 main Solution 2.naavrewf 0

# Laserfarm Virtual Lab

Scenario: map vegetation characteristics using LiDAR data.



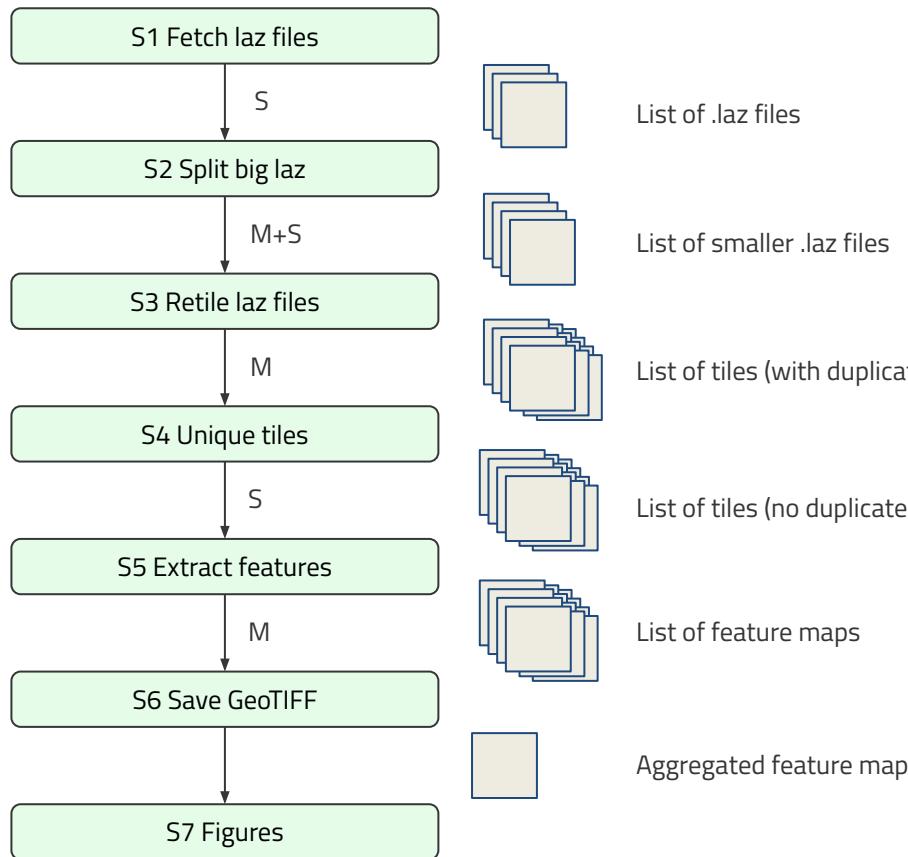
Yifang Shi



## 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



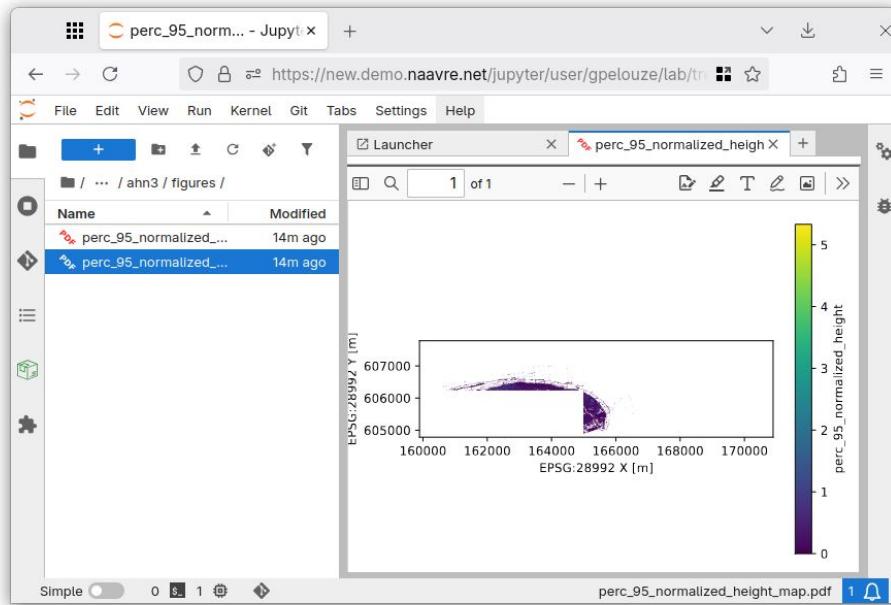
# Laserfarm workflow



# Laserfarm workflow results

**Getting the output:** open the file browser and go to:

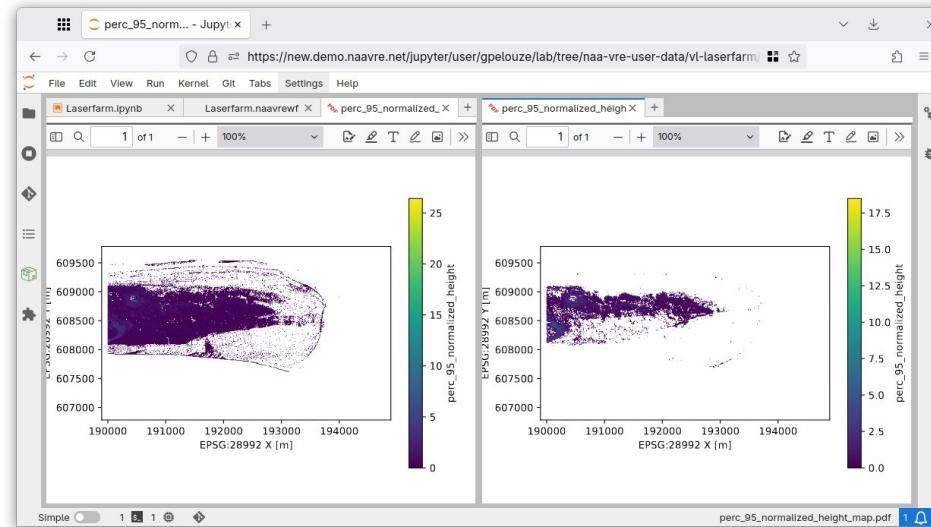
naa-vre-user-data/vl-laserfarm/small\_terschelling/ahn3/



**Other datasets:** explore values of  
param\_minio\_public\_dataset\_prefix:

vl-laserfarm / small\_terschelling / ahn3  
medium\_ameland / ahn4 /

**Other datasets:** change value of param\_feature\_name  
List: <https://laserchicken.readthedocs.io/en/latest/#features>





# THANKS!



UNIVERSITY  
OF AMSTERDAM

**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"



Finanziato  
dall'Unione europea  
NextGenerationEU



Ministero  
dell'Università  
e della Ricerca

