Notebook-as-a-VRE: collaborative virtual labs to build digital twins of ecosystems

Gabriel Pelouze[1,2], Spiros Koulouzis[1,2], Koen Greuell[1,2], Nafiseh Soveizi[2], and Zhiming Zhao[1,2]

vlic@lifewatch.eu, z.zhao@uva.nl

[1] LifeWatch ERIC, Virtual Lab & Innovation Center (VLIC), Amsterdam, The Netherlands
[2] Multiscale Networked Systems, University of Amsterdam, Amsterdam, The Netherlands

EGU25 – ESSI2.3 – 1 May 2024

Complexity of ecosystems
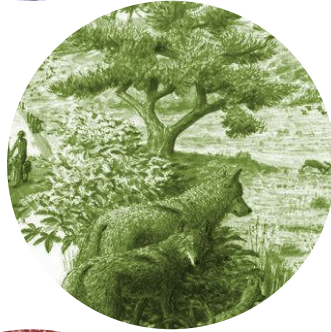
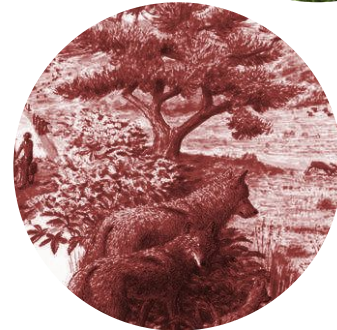# Digital twin for predictive studies

Physical system

Digital twin

Scenario 1

Scenario 2

Scenario 3

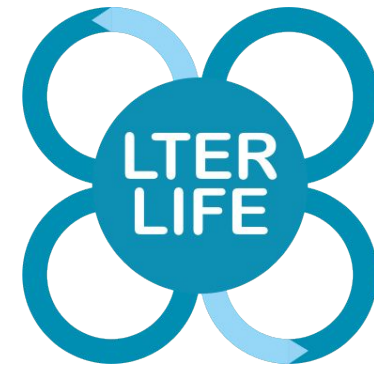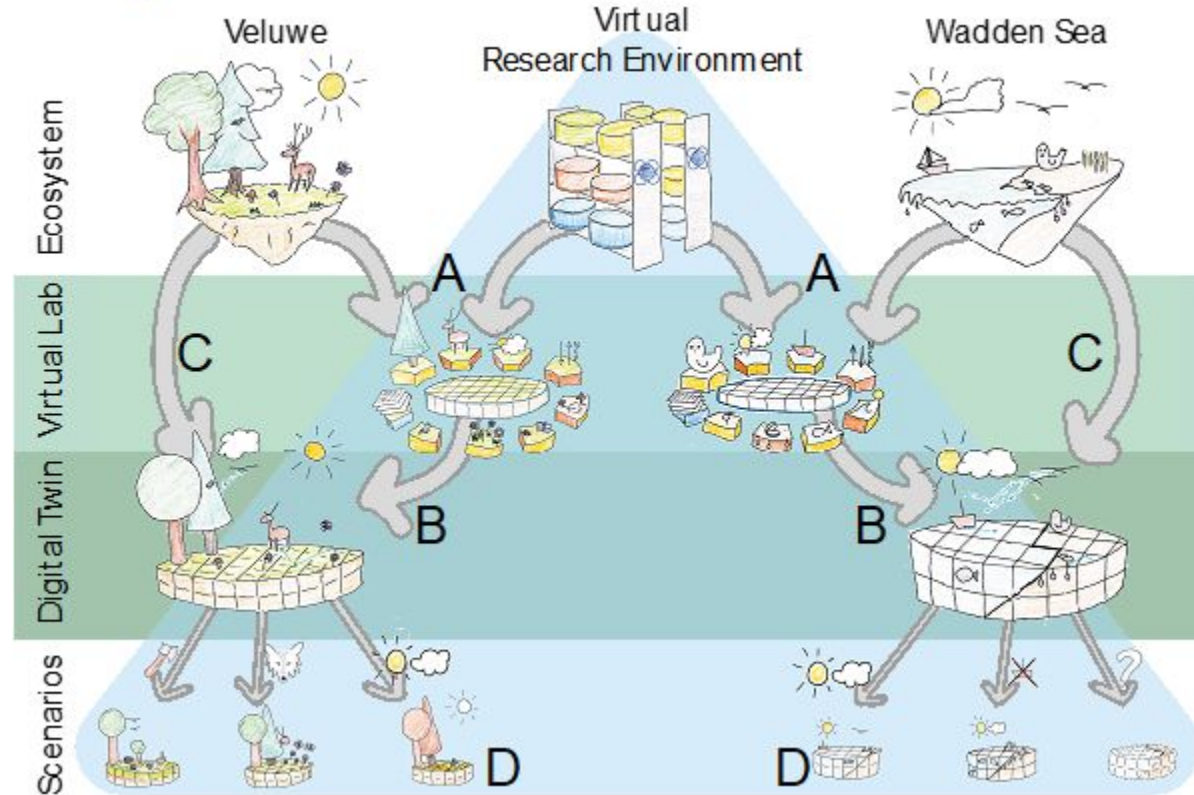# But... scattered data and models

LTER-LIFE: a Dutch DT infrastructure project

https://lter-life.nl/en

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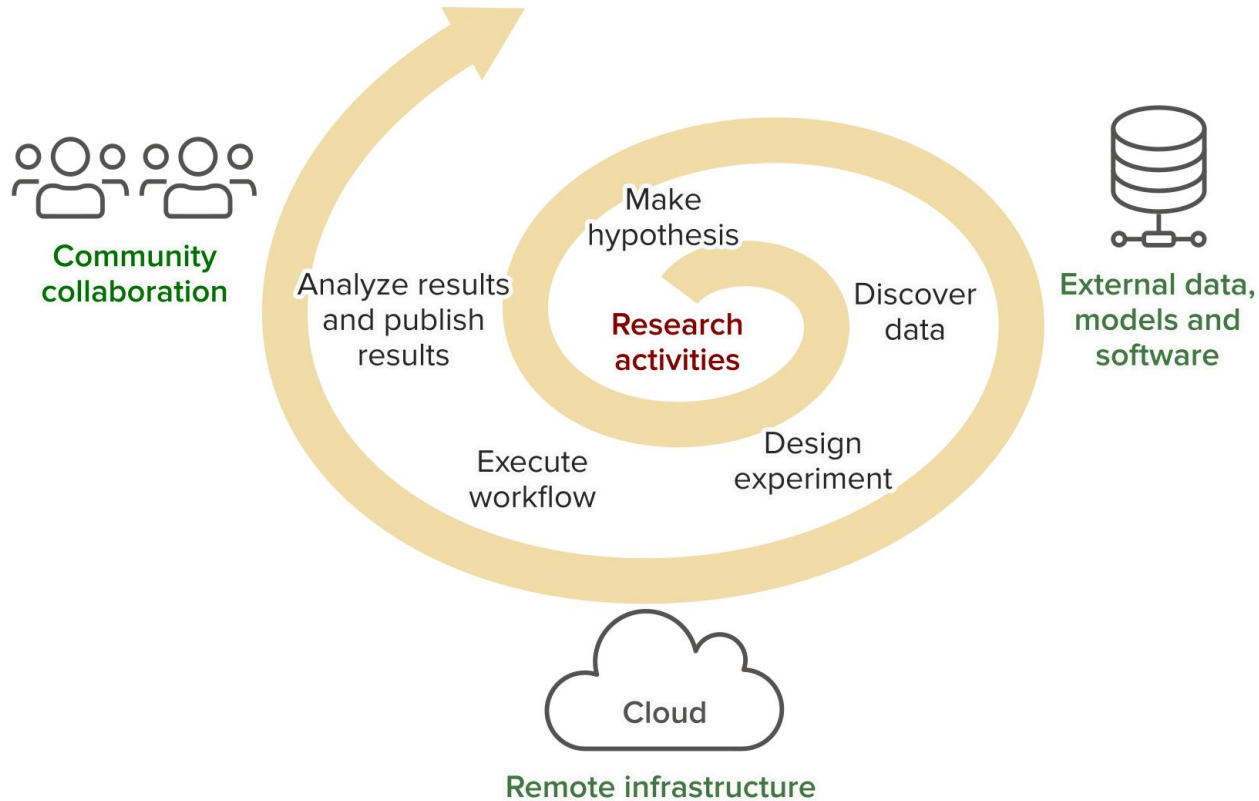
"Virtual Research Environments (VREs) provide user-centric support for discovering and selecting data and software services from different sources and composing and executing application workflows, ..." (Jeffery et al., 2020)

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**
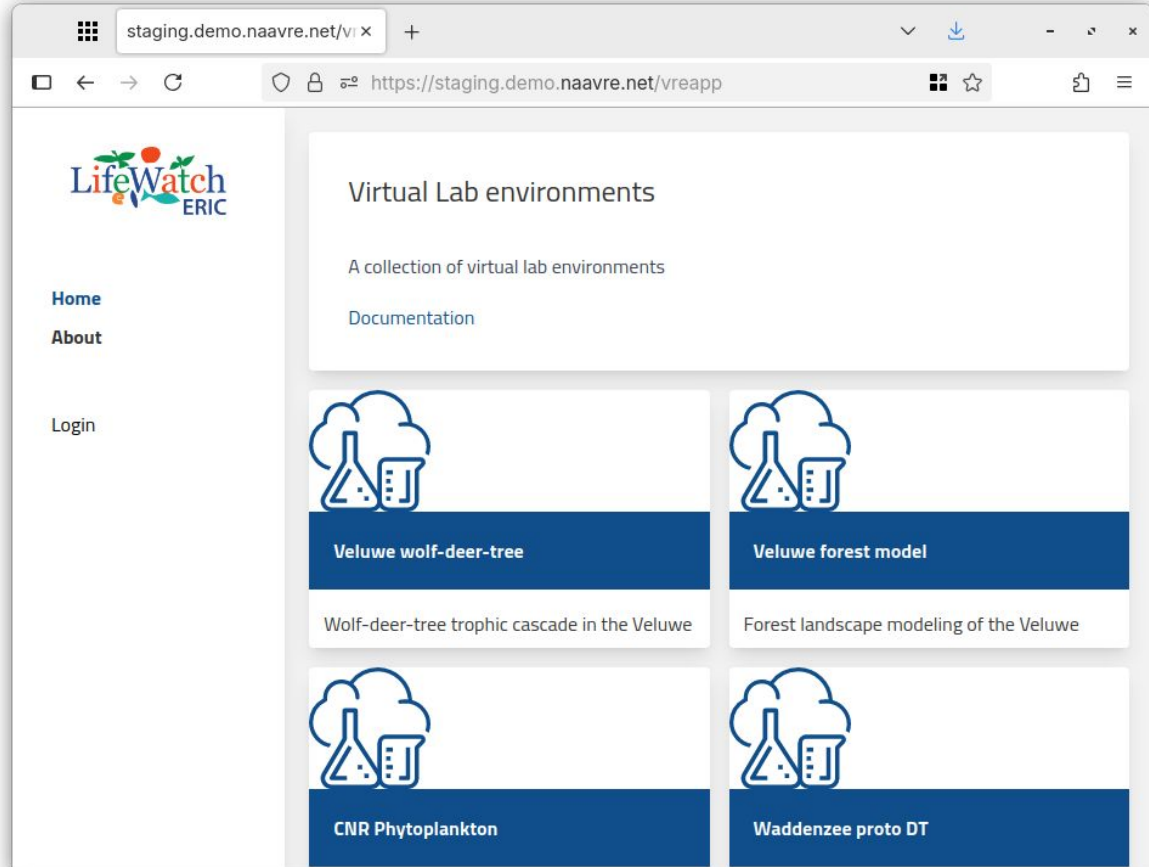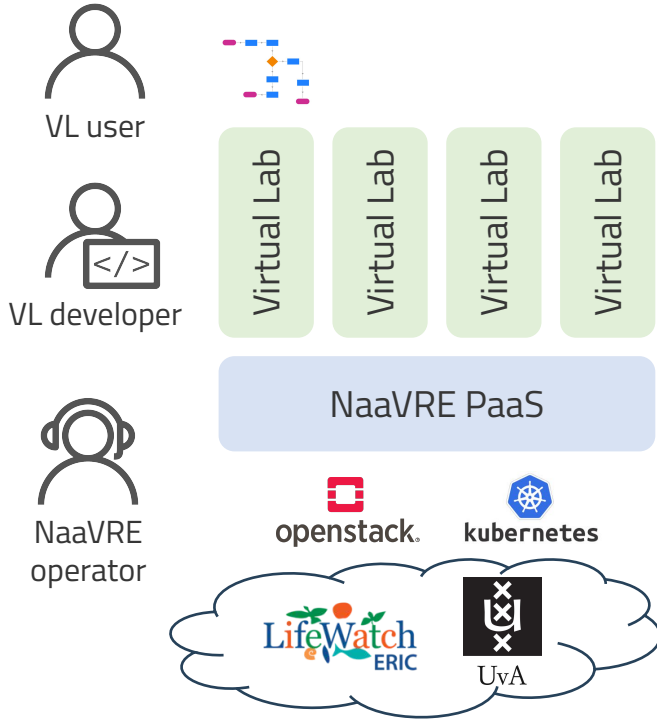
- **Combined, they are NaaVRE**
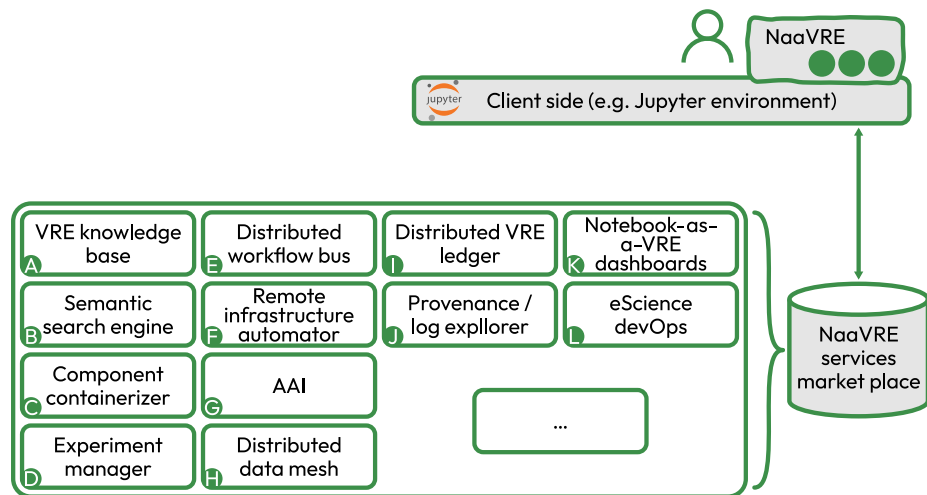
Research activities and Jupyter extensions
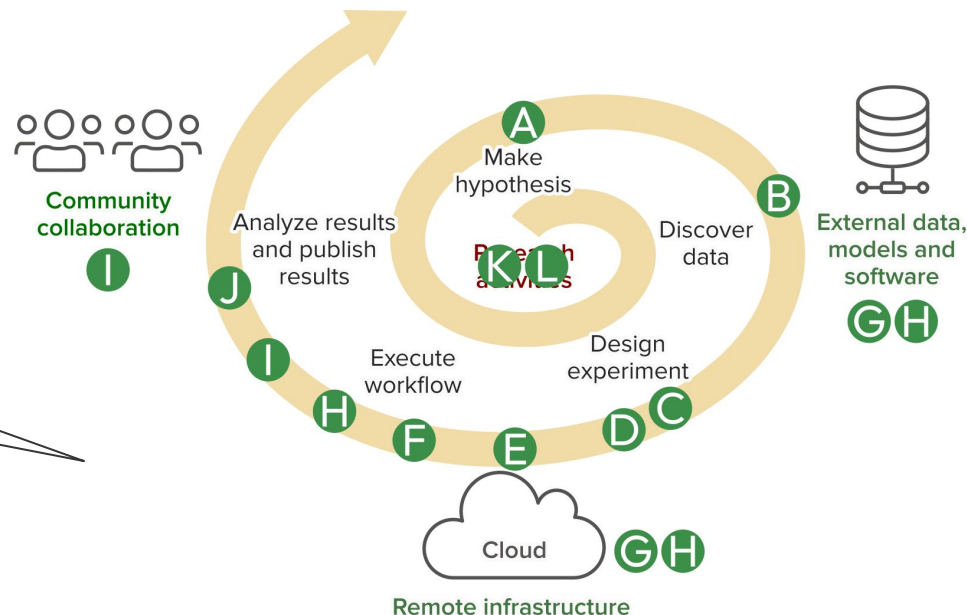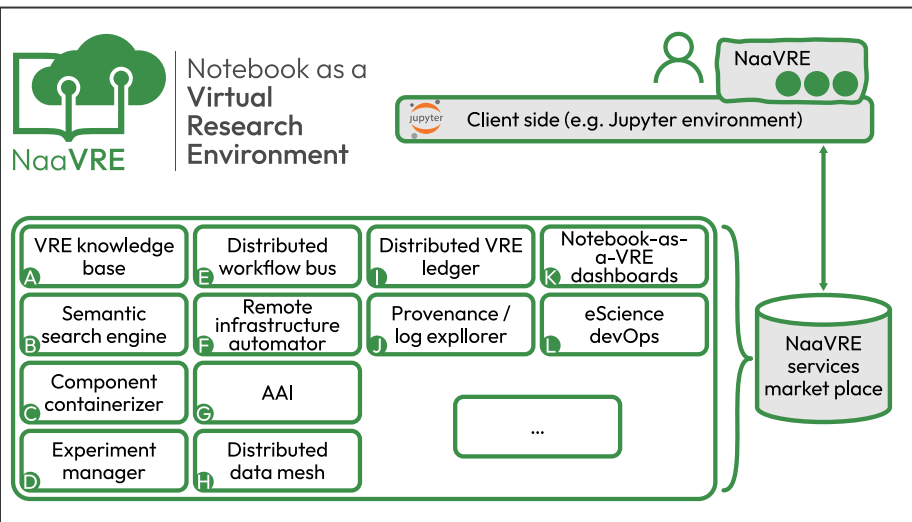
Zhao, Z., Koulouzis, S., Bianchi, R., Farshidi, S., Shi, Z., Xin, R., Wang, Y., Li, N., Shi, Y., Timmermans, J., Kissling, W.D.: Notebook-as-a-VRE (NaaVRE): From private notebooks to a collaborative cloud virtual research environment. Softw Pract Exp. spe.3098 (2022). https://doi.org/10.1002/spe.3098.
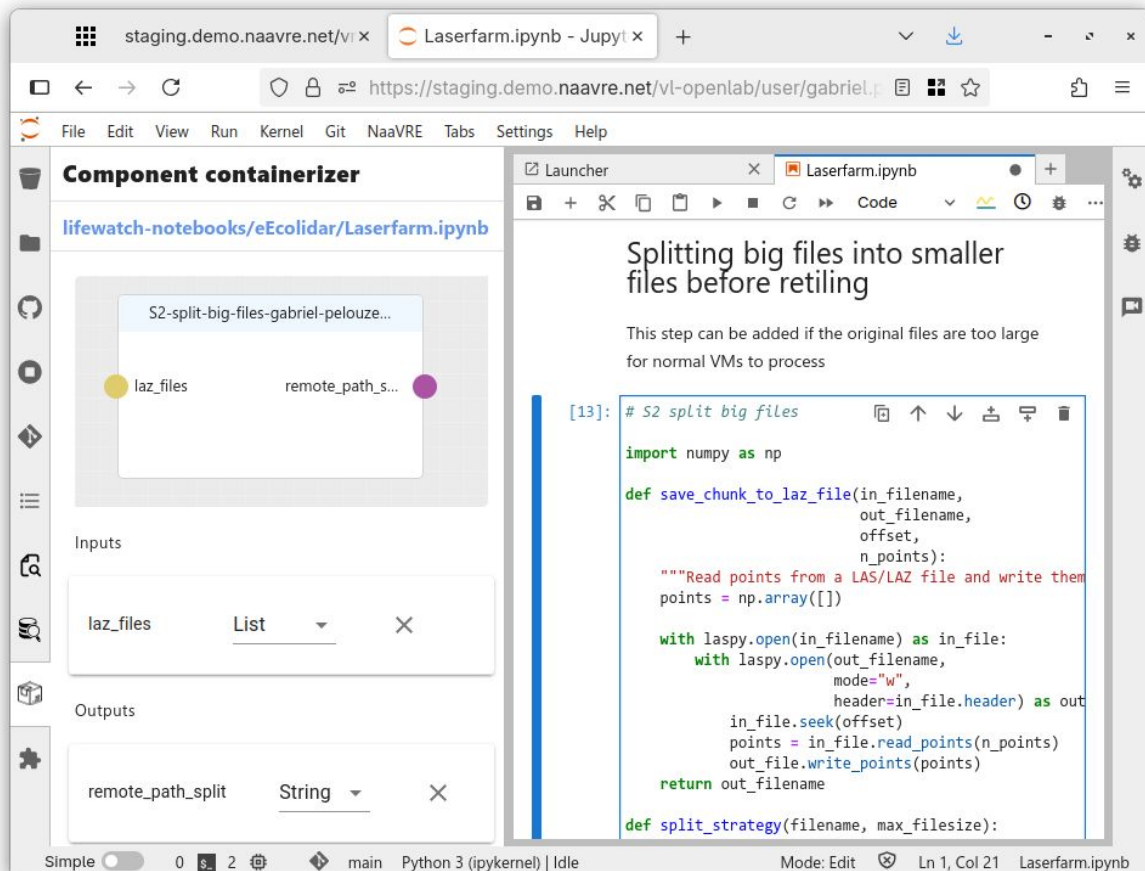
Notebook-as-a-VRE and Virtual Labs

From notebooks to cloud workflows

1. PROTOTYPE MODEL IN NOTEBOOK
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
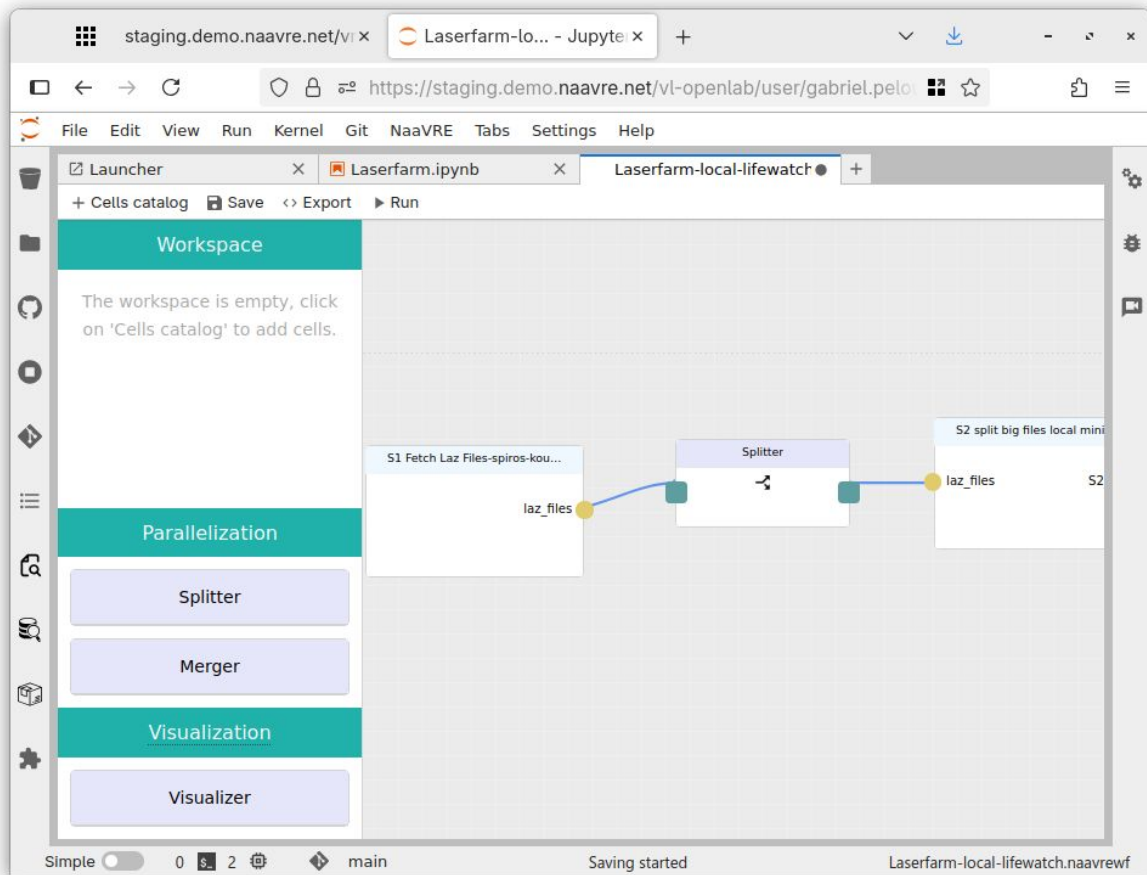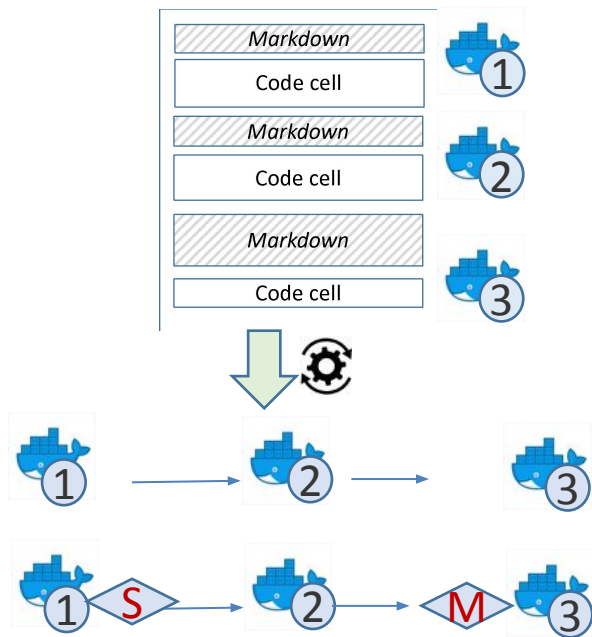
From notebooks to cloud workflows

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

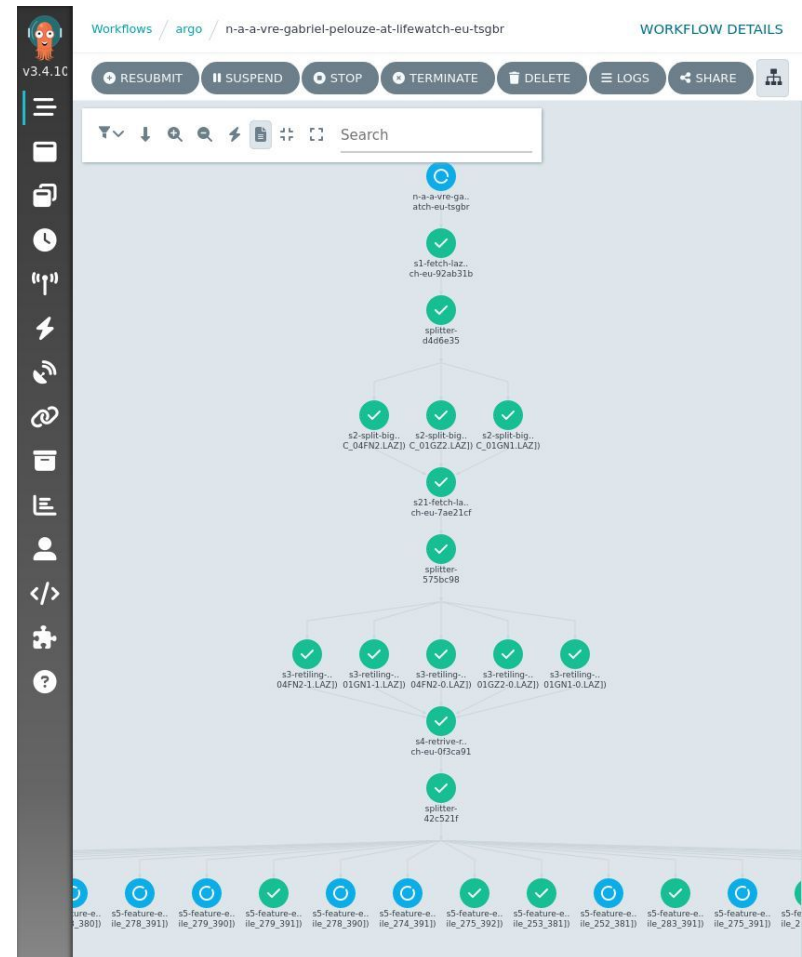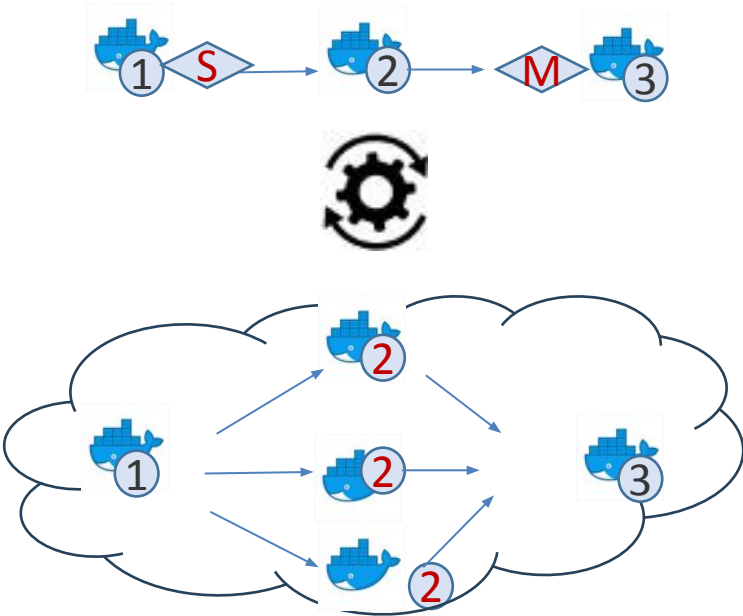Zhou, H., Hu, Y., Ouyang, X., Su, J., Koulouzis, S., Laat, C., Zhao, Z.: CloudsStorm: A framework for seamlessly programming and controlling virtual infrastructure functions during the DevOps lifecycle of cloud applications. Softw: Pract Exper. 49, 1421–1447 (2019). https://doi.org/10.1002/spe.2741

VRE and Virtual Lab co-development framework
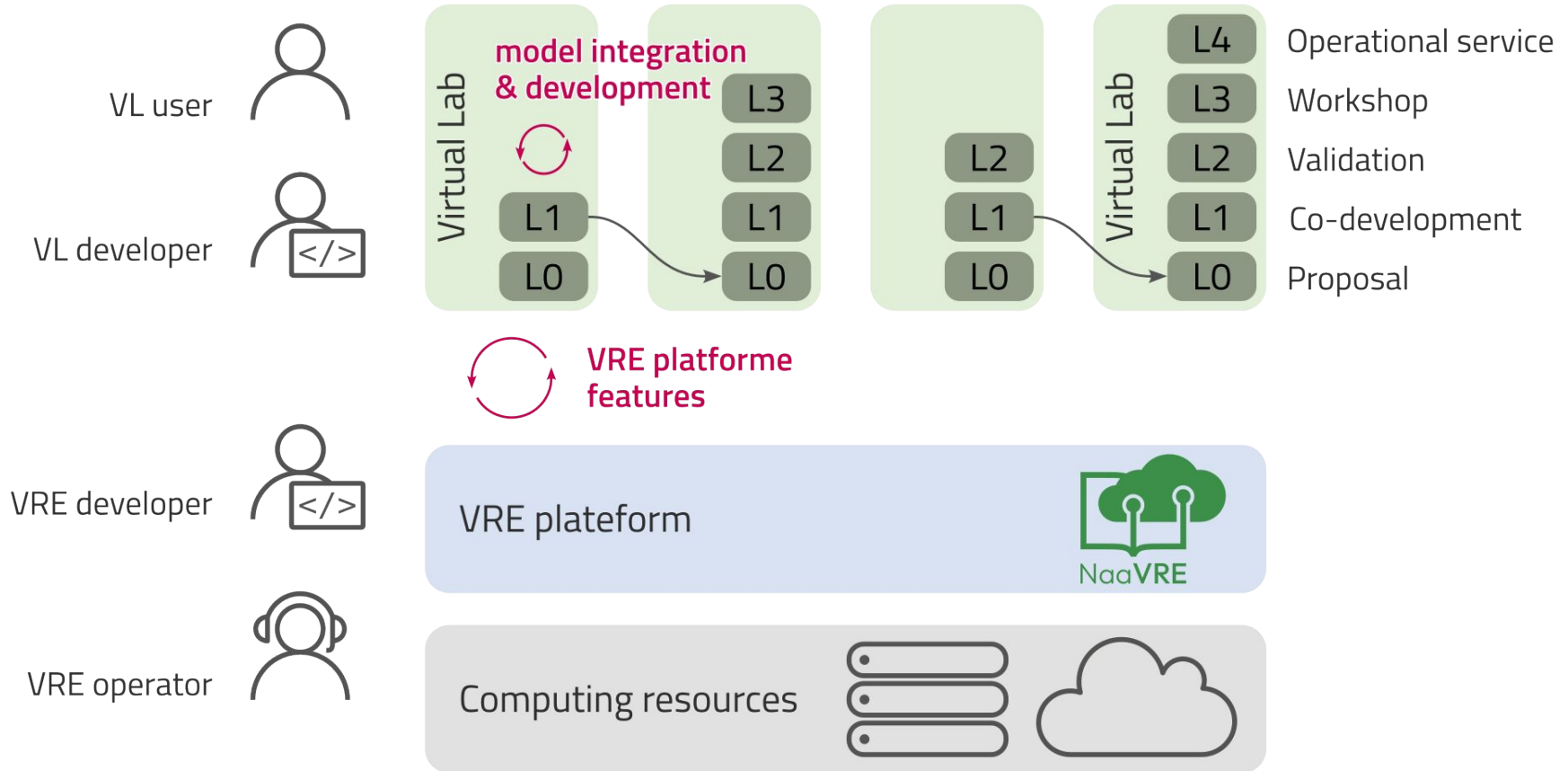
Digital Twin Virtual Labs

- Veluwe (forest)
    - Bud burst prediction
    - Forest model
    - Wolf-deer-tree
      trophic interaction
- Waddenzee
  (intertidal zone)
    - Remote sensing of
      primary production

FAIR Data & Models

Community

Virtual Lab

LTER LIFE
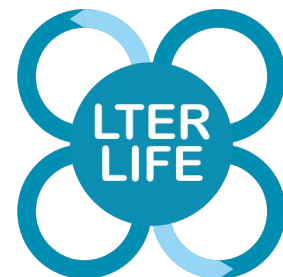
Digital-twin oriented developements and open challenges

Digital-twin

- Model and data FAIRification
- Model composition and runtime integration ("DT engine")
- AI in digital twins (e.g. knowledge graphs, machine learning, fundation models)

Supporting

- FAIR Digital Objects (RO-crate)
- Community engagement
- Software quality

See for yourself

https://naavre.net

Learn, try, get in touch