Digital Twin of aquatic ecosystem and its needs for FAIR data & model

Qing & Lisette, GLEON workshop, 16/02/2025

Practical information:

- mentimeter will be used for the interactive parts of the workshop and getting input from you
- The workshop consists of (1:30 - 4:30):

  1:30 - 2:00 Presentations about Digital twin By Qing

  2:00 - 2:15 Discussion

  2:15 - 2:30 Break

  2:30 - 2:45 FAIR data by Lisette

  2:45 - 3:00 Discussion

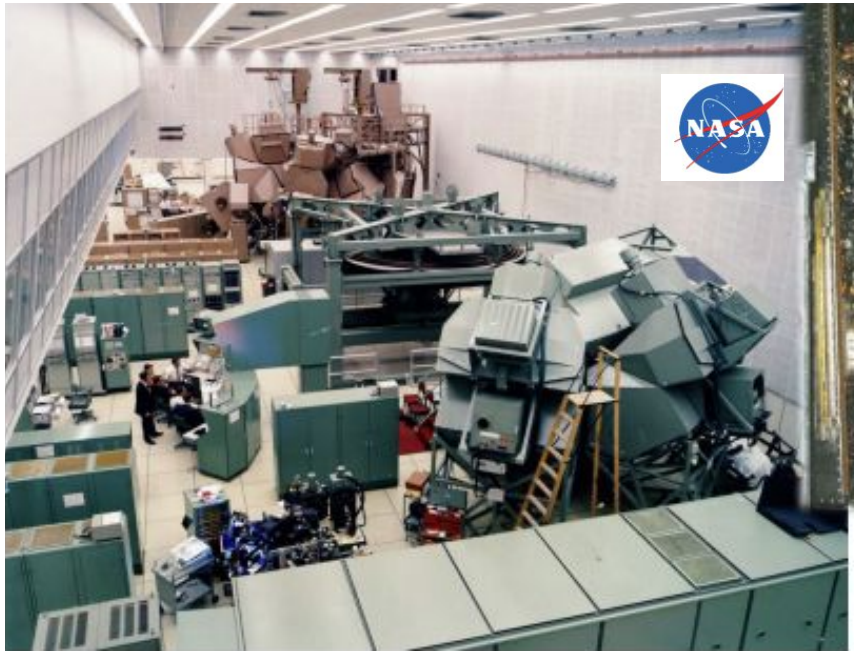
  3:00 - 3:30 Coffee-break

  3:30 - 3:45 Introduction of Hands-on session (by Qing)

  3:30 - 4:30 Hands-on session: running PCLake in cloud

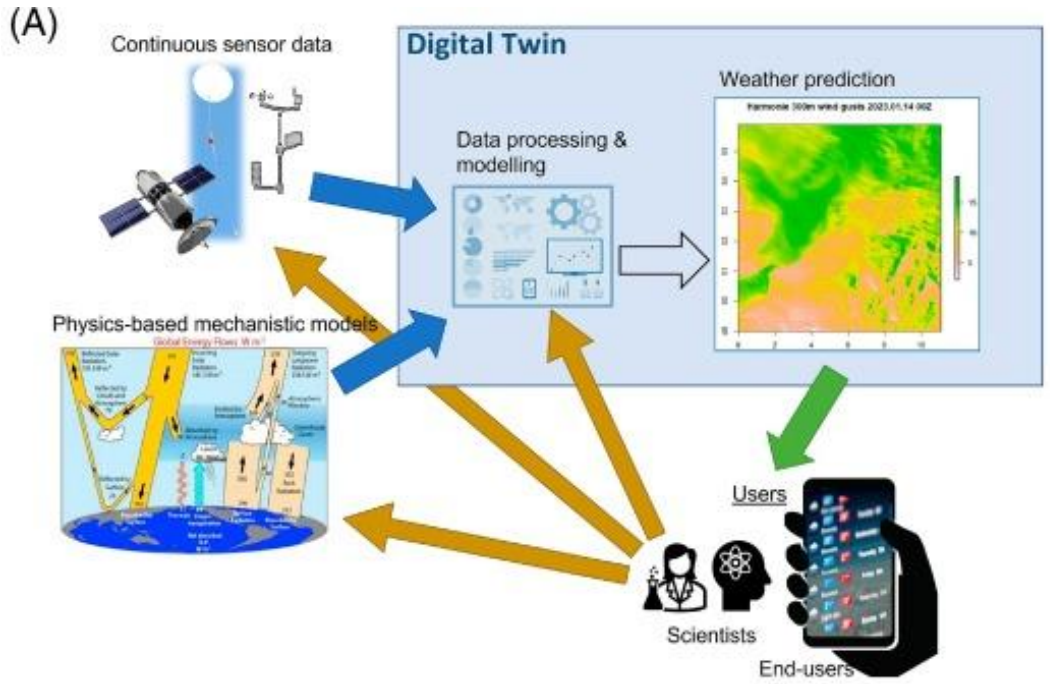
History of digital twin

- (**Physical**) Twin: NASA uses simulators, as part of the Apollo 13 mission, to train astronauts and mission controllers.
- **Digital** Twin: Digital **replica** of a physical entity, allowing users to **predict interactions** & **responses** to external drivers.

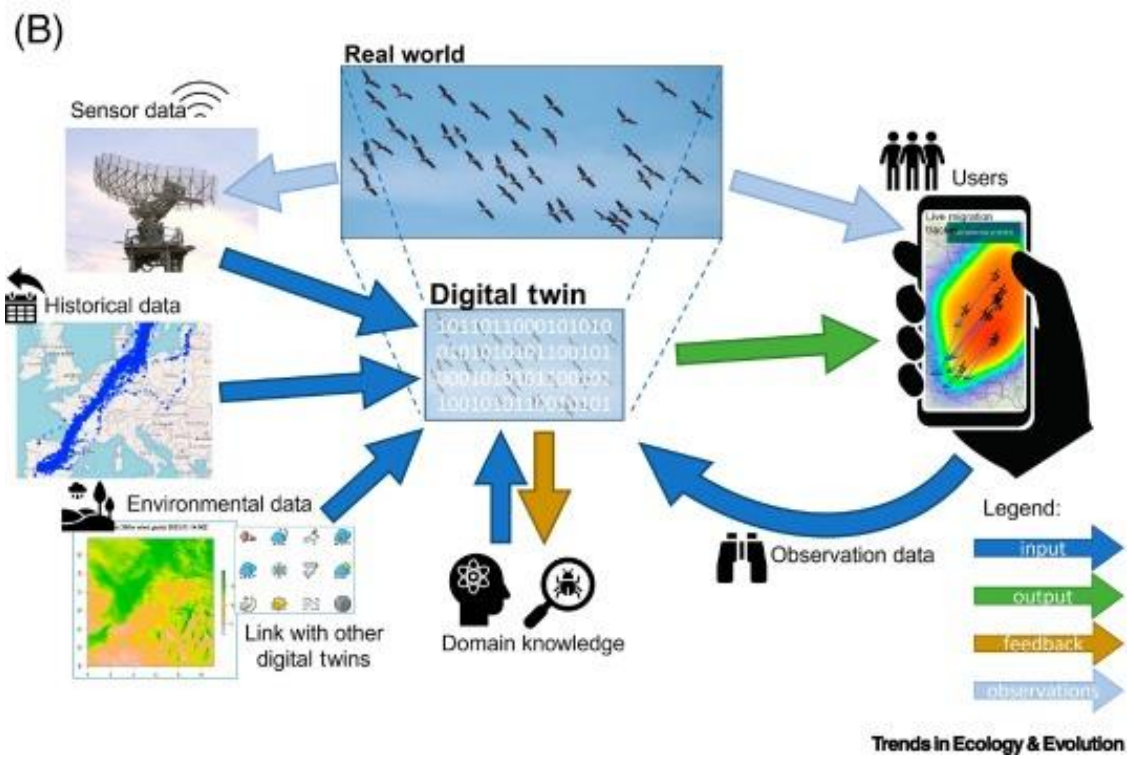


Digital twin example in natural environmental science

Weather forecast



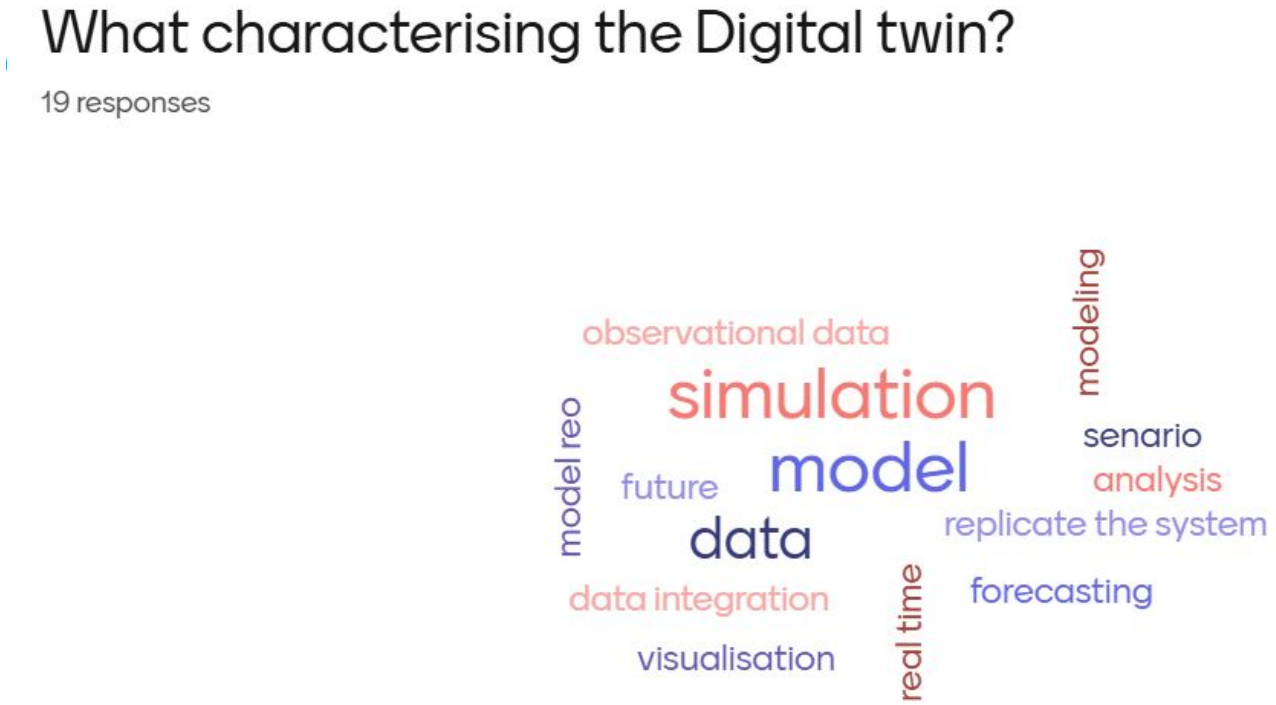
Crane migration



De Koning et al. 2023; Digital twins: dynamic model-data fusion for ecology

Characteristics of ecosystem digital twin

Open mentimeter.com and share your thoughts (code: **6489 0193**)



Catalogues of assets

Model

Model

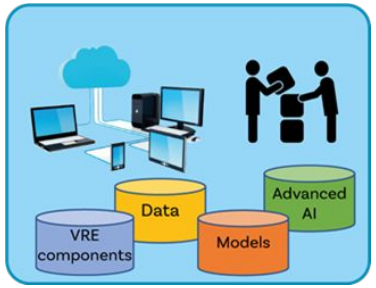
Tool

Tool

Data

Expertise

Virtual Research Environment

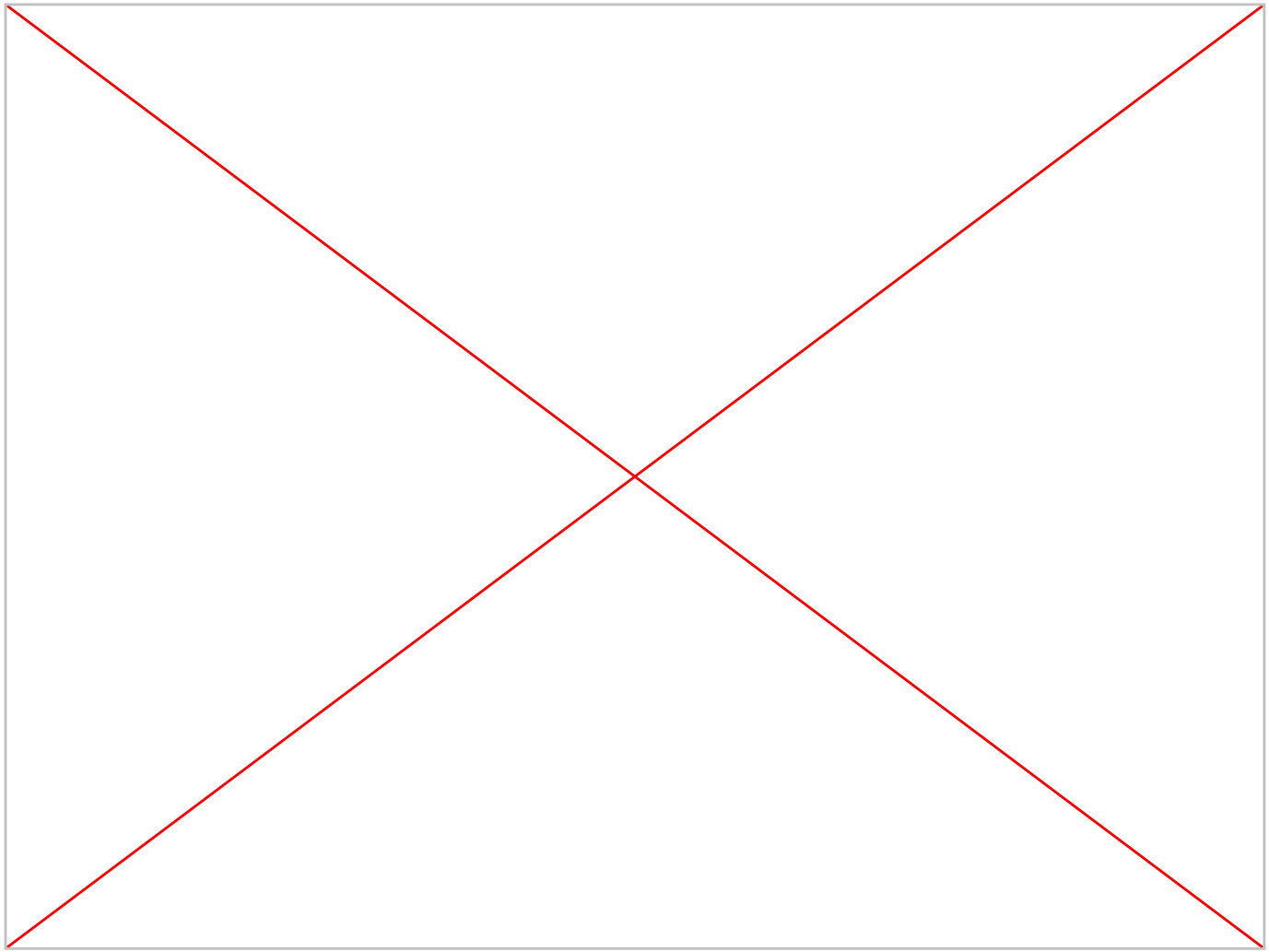


Digital Twins

scenarios

predictive ecology

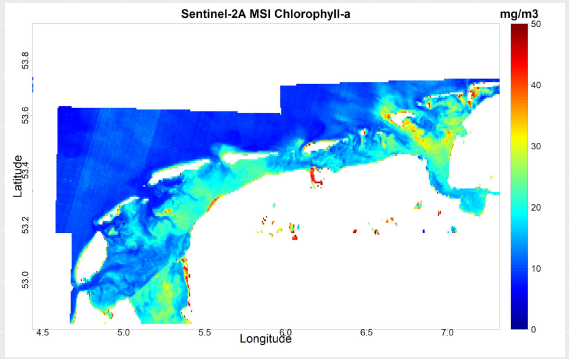
Example use case: Building workflow for Primary Production



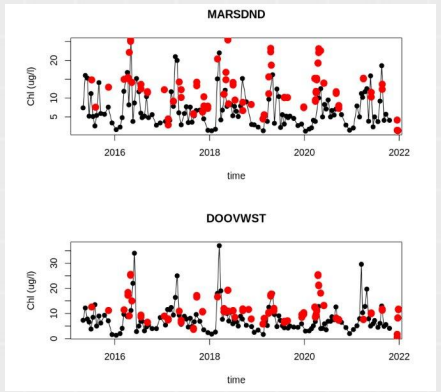
Workflow for assessing Primary production

Raw satellite image

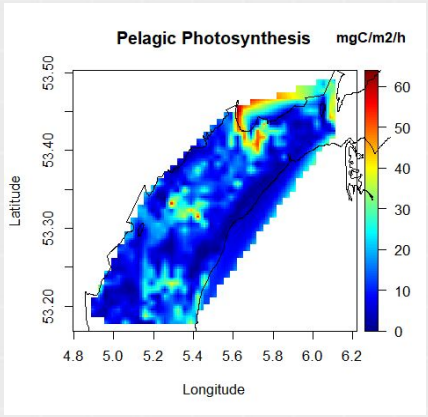
Chl-a processing

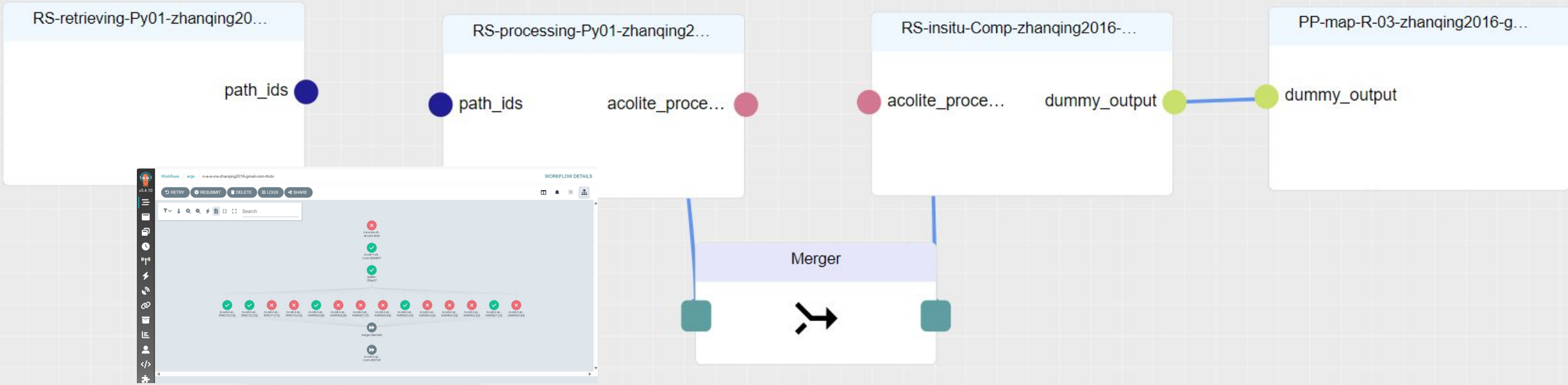


In-situ vs remote sensing



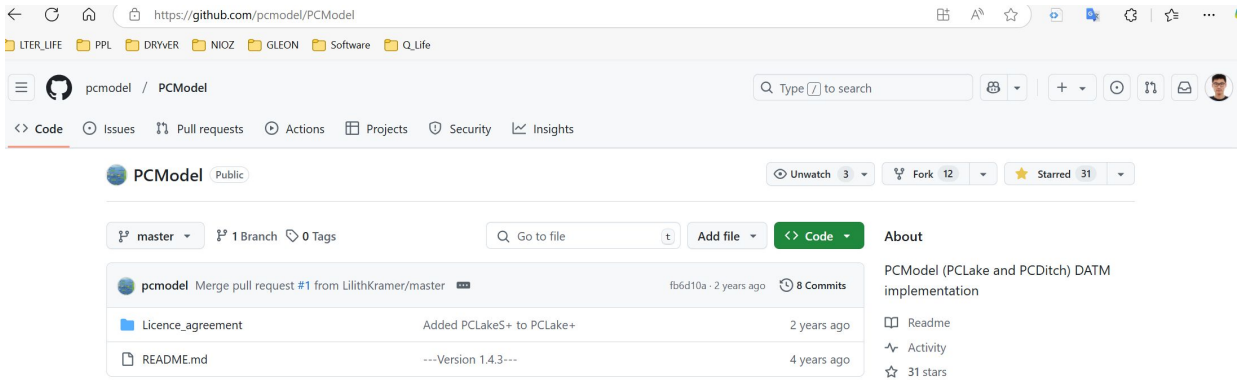
Primary production

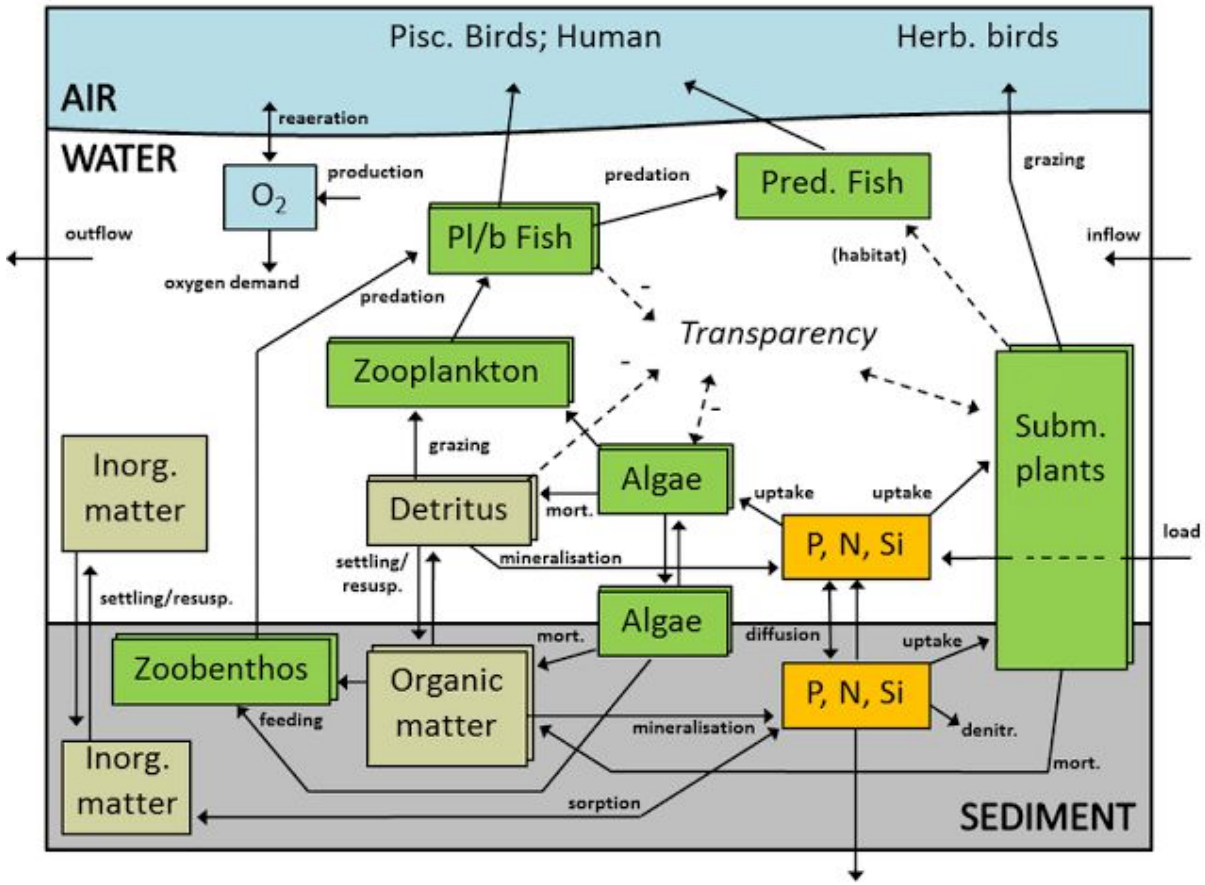




Use case: Running PCLake on cloud

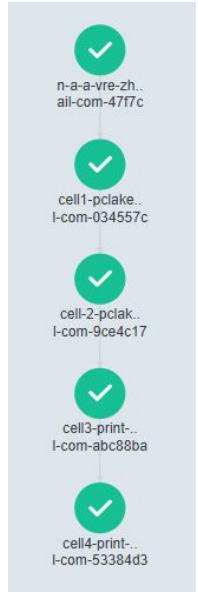
- PCLake is a process-based ecosystem model
- It models nutrient cycle and biomass-based foodweb
- It is open! But FAIR?



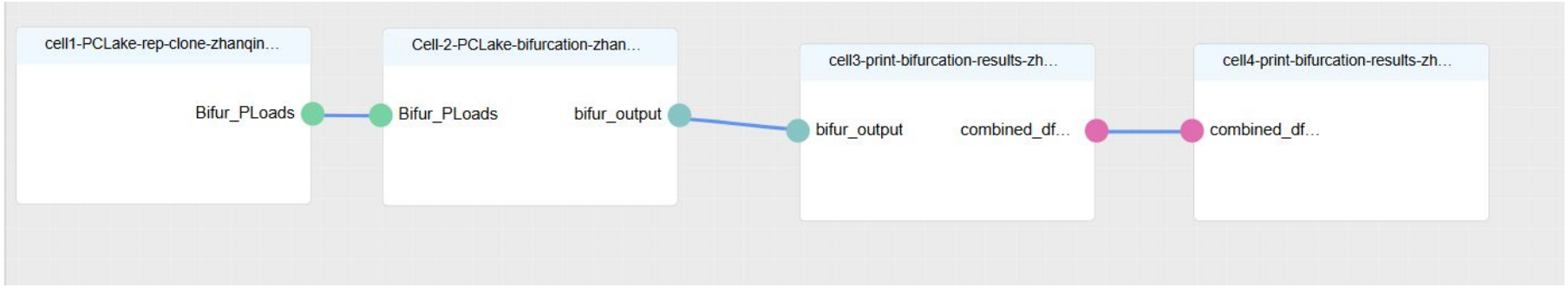


Hands-on: Running PCLake on cloud

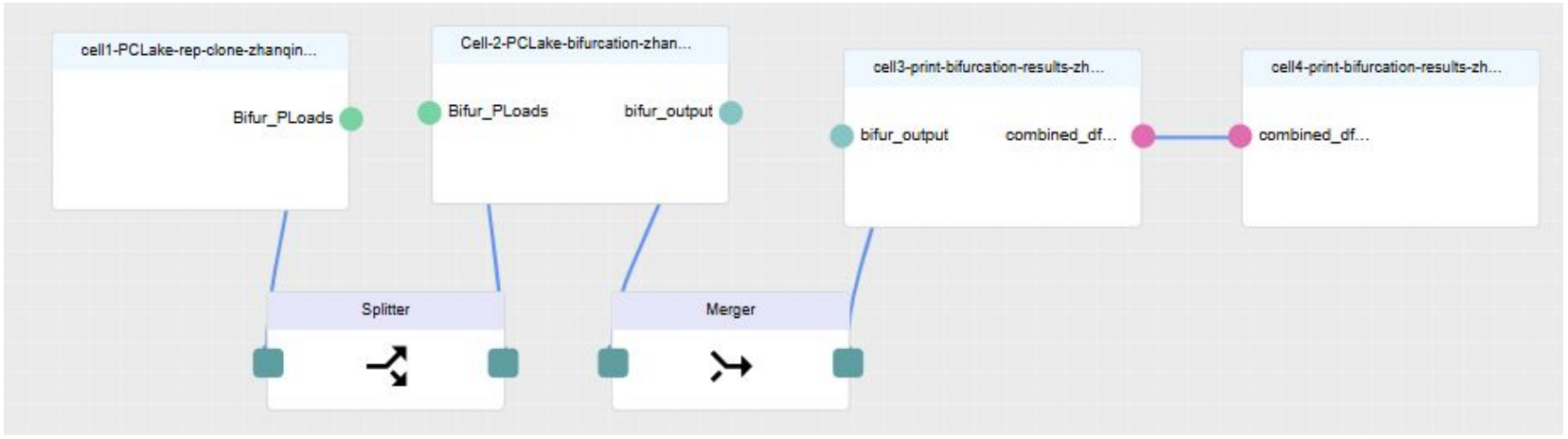
Workflow structure



Sequential:



Parallel:



Pros & Cons of using the e-infrastructure

Advantages?

Limitations?

FAIR Data & Models

Findable Accesible Interoperable Reusable

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Open

Virtual Lab

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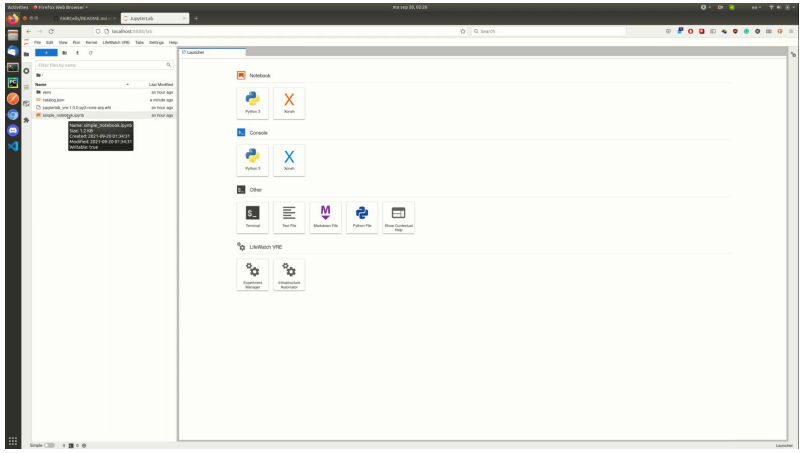
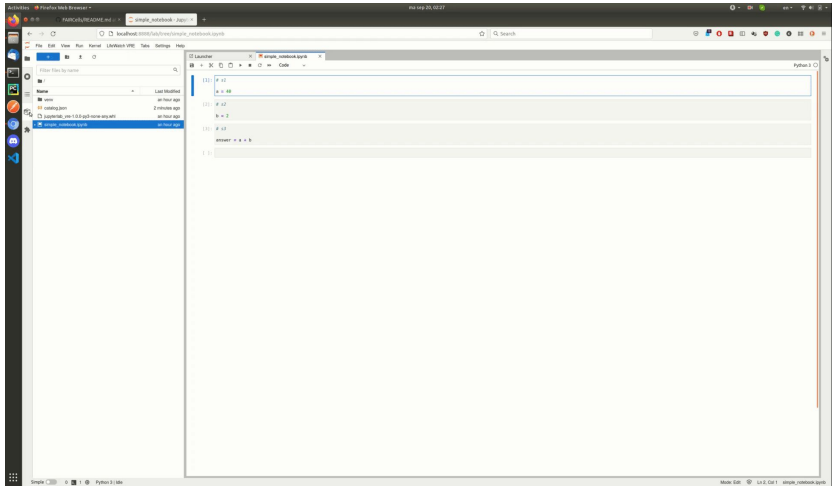
Running Workflows in the Cloud in 4 Steps

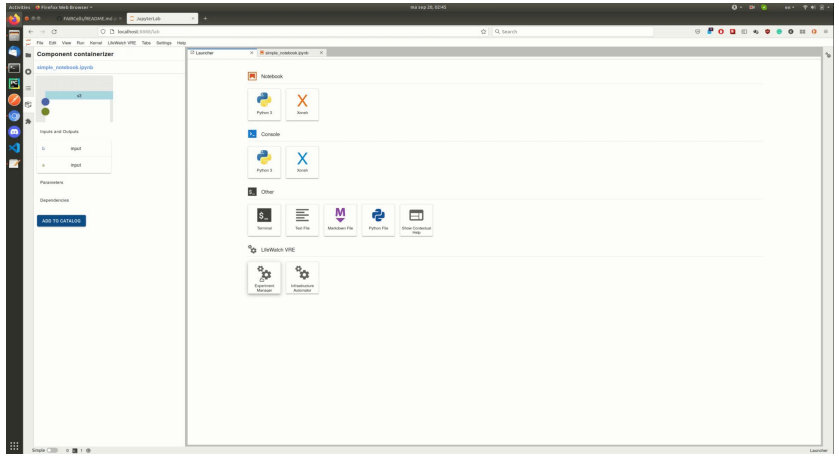
1. Prototype code in Jupyter



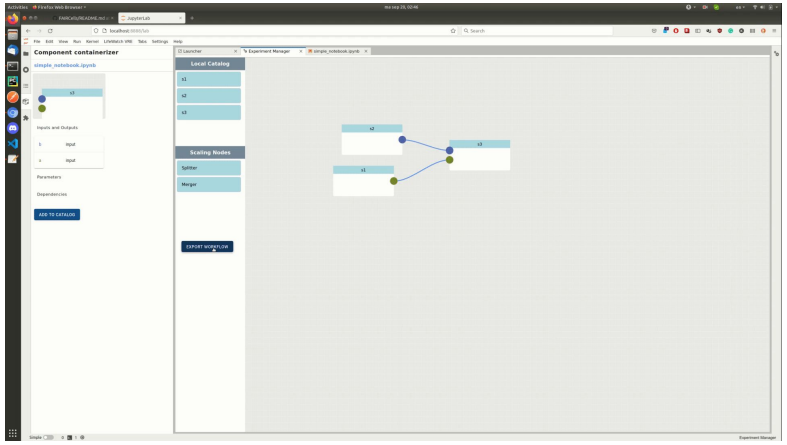
2. Containerize Cells



3. Compose Workflow



4. Execute Workflow



Steps:

1. Go to: https://naavre.lifewatch.dev/vreapp
2. Choose lab: Wadden_proto_DT
3. Upload files from github: NIOZ-QingZ/GLEON2025_Workshop_DT: Digital Twin Workshop GLEON2025. R & Python Notebooks.

Authorization keys needed

param_s3_server = "scruffy.lab.uvalight.net:9000"

param_s3_public_bucket = "naa-vre-waddenzee-shared"

param_s3_public_prefix = "vl-waddenzee-proto-dt"

param_s3_user_bucket = "naa-vre-user-data"

Get your own:

param_s3_user_prefix = ""

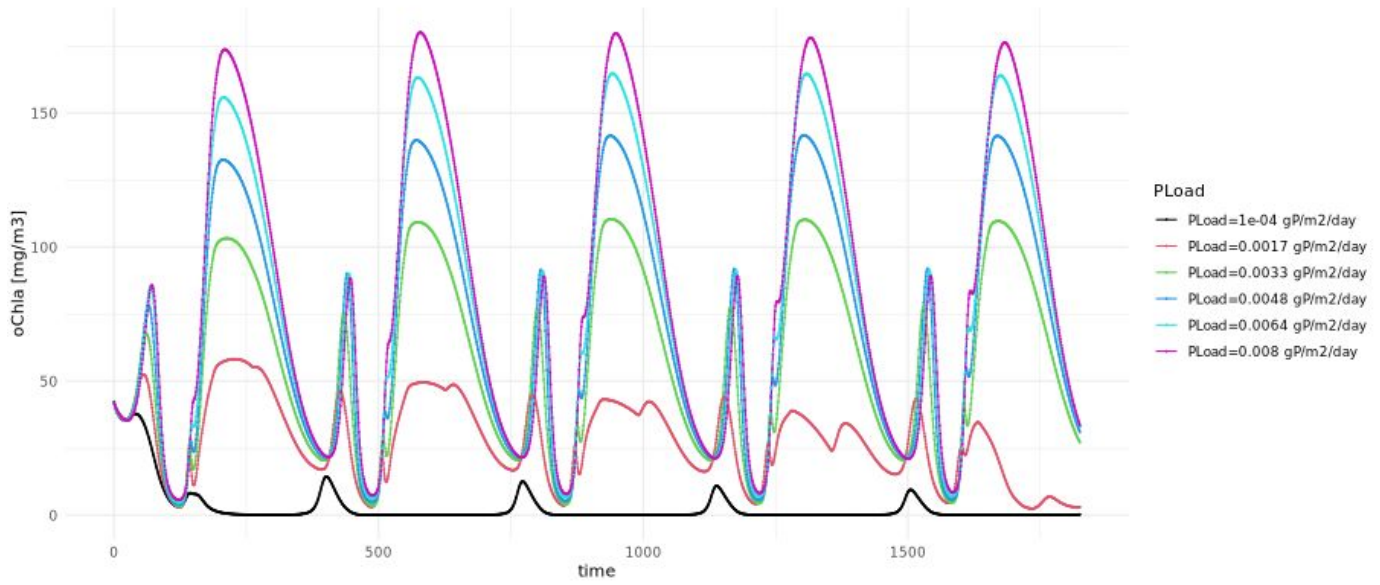
secret_s3_access_key = ""

secret_s3_secret_key = ""

Bifurcation analysis results:

Chla levels under different phosphorus loadings

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
PLoad	nParamSe	nStateSet	time	sPO4W	sO2W	sDDiatW	sDZoo	sDFiAd	sDVeg	sDBent	oPTotW	oChla	aSecchi	aDError	aNError	aPError	
1.00E-04	1	1	0	0.01	10	0.5	0.05	2	1	1	0.055	42.22338	0.780142	-7.28E-12	-5.68E-14	0	
1.00E-04	1	1	1	0.005996	10.73726	0.484898	0.051285	1.996805	0.992939	1.004458	0.058114	41.30182	0.789281	1.46E-11	-2.27E-13	-1.55E-10	
1.00E-04	1	1	2	0.004315	11.31441	0.474853	0.052527	1.993645	0.986508	1.008881	0.061138	40.5298	0.797313	1.46E-11	-4.26E-13	-5.29E-10	
1.00E-04	1	1	3	0.003771	11.76948	0.468778	0.053733	1.990517	0.980265	1.013267	0.064066	39.86461	0.804583	2.18E-11	-6.54E-13	-9.80E-10	
1.00E-04	1	1	4	0.003749	12.13002	0.465899	0.054912	1.987421	0.974175	1.017618	0.066904	39.28359	0.811252	2.18E-11	-7.67E-13	-9.15E-10	
1.00E-04	1	1	5	0.003985	12.41735	0.465665	0.056069	1.984354	0.968232	1.021933	0.069661	38.77047	0.817437	1.46E-11	-9.95E-13	-1.51E-09	
1.00E-04	1	1	6	0.004341	12.6496	0.46769	0.057209	1.981317	0.962432	1.026212	0.072335	38.31354	0.823219	1.46E-11	-1.39E-12	-1.82E-09	
1.00E-04	1	1	7	0.004911	12.83862	0.471701	0.058339	1.978307	0.956776	1.030457	0.074927	37.90425	0.828658	-7.28E-12	-1.93E-12	-2.92E-09	
1.00E-04	1	1	8	0.005722	12.99324	0.477358	0.059462	1.975324	0.951259	1.034667	0.07744	37.5349	0.83381	0	-3.55E-12	-7.38E-09	
1.00E-04	1	1	9	0.006791	13.12085	0.484558	0.060585	1.972367	0.945883	1.038844	0.079878	37.20128	0.838699	-1.46E-11	-2.93E-12	-6.61E-09	
1.00E-04	1	1	10	0.008118	13.22735	0.493294	0.06171	1.969435	0.940643	1.042988	0.082243	36.90083	0.843332	0	-2.61E-12	-5.80E-09	
1.00E-04	1	1	11	0.009683	13.31729	0.503566	0.062844	1.966526	0.935538	1.047101	0.084541	36.63016	0.847721	-7.28E-12	-2.44E-12	-5.56E-09	



Group Task: relationship between parallel branches and running time

Structure (Sequential OR Parallel)	Scenarios (1-10)	Contributor (Your Name)	Computing time (mins)
Sequential	3		
Parallel	3		
Sequential	5		
Parallel	5		
Sequential	10		
Parallel	10		
Sequantial	20		
Parallel	20	Qing	55

Pros & Cons of using the e-infrastructure

Open mentimeter.com and provide your feedbacks (code: **6489 0193**)

Advantages?

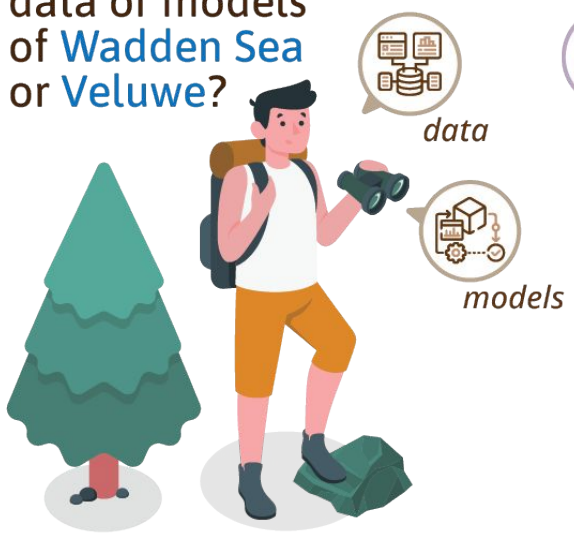
- It resolves a common issue: "it works on my computer..."
- Interoperable
- Easier to scale up
- Execution not limited to sequential order (speed up by parallelization)

Limitations?

- Overhead (slower for smaller computation task)
- Capacity-building needed for start user (certain level of understanding on architecture of the infrastructure)
- Stable internet connection (Crucial!)

Join the community!

Do you have data or models of Wadden Sea or Veluwe?



Do you want to build a Digital Twin?

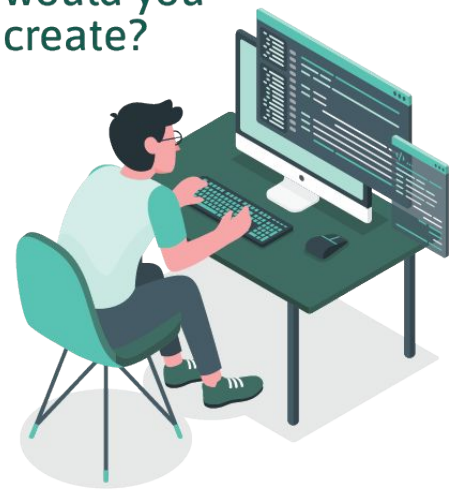
SCAN ME

https://lter-life.nl/en

lter-life@nioo.knaw.nl

You can help!

What digital twin would you create?



What should the virtual lab look like?

Drawings by Geerten Hengeveld
Design by Stefan Vriend, Geerten Hengeveld
using illustrations from Storyset, Freepik, Flaticon

LTER-NL Netherlands Long-term Ecosystem Research Network
LifeWatch ERIC
NIOO
NIOZ
Rijksinstituut voor Volksgezondheid en Milieu
Ministerie van Volksgezondheid, Welzijn en Sport
Universiteit van Amsterdam
Wageningen University & Research
SURF
DANS
netherlands eScience center
NWO

Materials

Some materials:

- Getting Started with NaaVRE tutorial | NaaVRE
- 2024-02-19 NaaVRE S3 - Google Slides
- https://forms.gle/6wjCxT6sUun4sqUt6
- Digital_Twin_GLEON25 – Mentimeter
- https://naavre.lifewatch.dev/vl-waddenzee-proto-dt
- NIOZ-QingZ/GLEON2025_Workshop_DT: Digital Twin Workshop GLEON2025. R & Python Notebooks.
- n-a-a-vre-zhanqing2016-gmail-com-xw7j4 / argo / Workflows – Argo