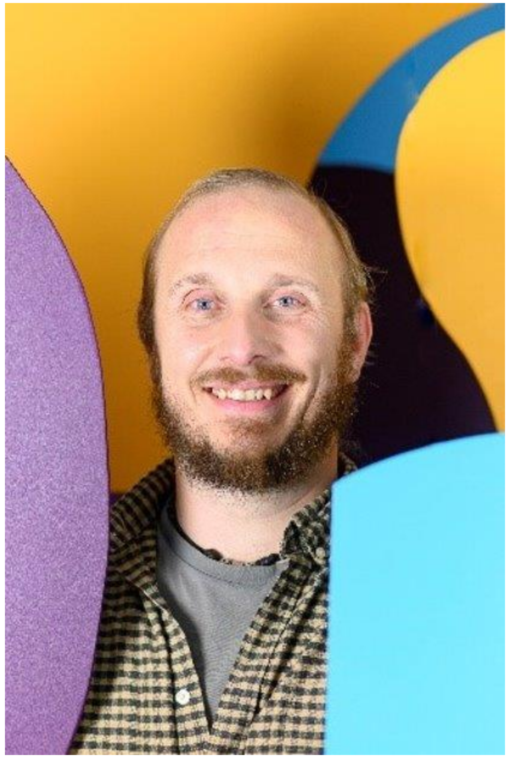
Interactive Geospatial Analysis at HPC scales: An Introduction to RS-DAT

netherlands eScience center

HDCRS Summer School, Reykjavik, 31-05-2023

SURF

People



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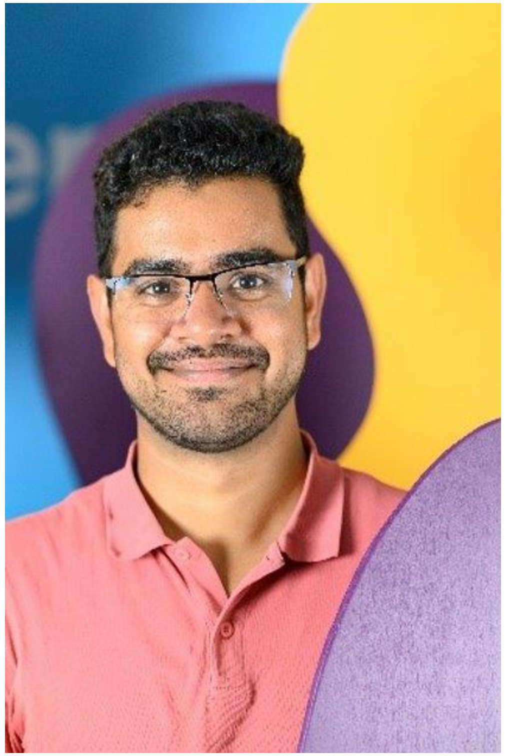

Pranav Chandramouli
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Housekeeping

https://tinyurl.com/2023-05-31-hdcrs

Schedule

09:00 – 10:30		**RS-DAT: EO stack on HPC**
	09:00	Intro/Housekeeping
	09:15	SURF/SPIDER – National HPC in NL
	09:25	RS-DAT, HPC, and the EO software ecosystem
	09:45	Deploying RS-DAT for HDCRS (hands-on)
	10:00	Dask (geospatial) (hands-on)
10:30 – 11:00		**Coffee**
11:00 - 12:00		**Data Retrieval**
	11:00	Intro to STAC and dCache
	11:15	Hands-on data retrieval
12:00 – 13:30		**Lunch**
13:30 – 15:00		**Scaling EO workflows**
	13:30	Hands-on workflow scaling
15:00 – 15:30		**Coffee**
15:30 – 17:00		**Deploying RS-DAT, Wrap up, Discussion**
	15:30	RS-DAT on “local” HPC
	15:30	Wrap up hands-on sessions
	16:15	Feedback/Disscussion
	<17:00	End

netherlands eScience center

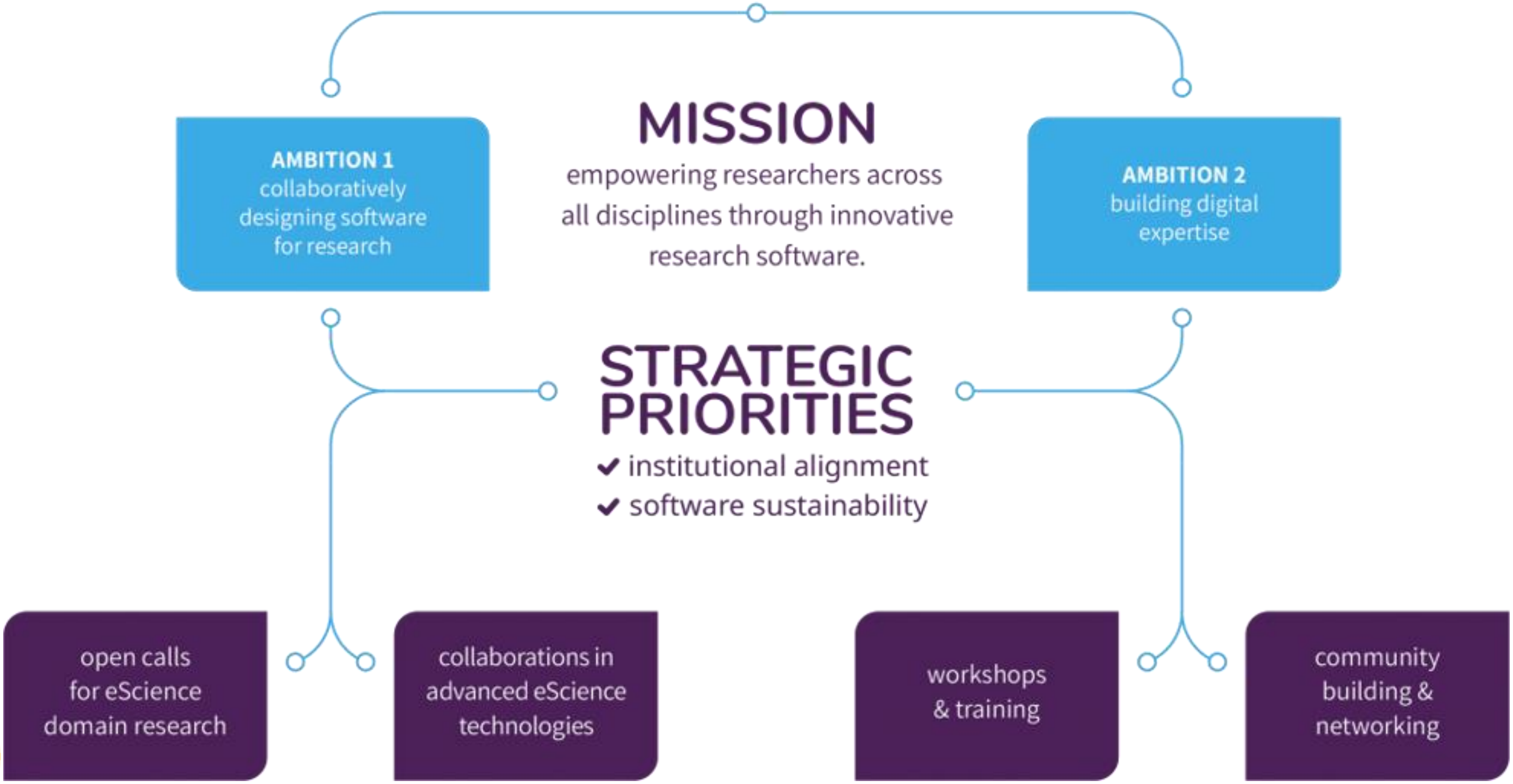
“Empowering researchers across all disciplines through advanced research software”

The Netherlands eScience Center

National centre / independent foundation since 2012 /

NWO & SURF

SURF NWO



AMBITION 1
collaboratively designing software for research

MISSION

empowering researchers across all disciplines through innovative research software.

AMBITION 2
building digital expertise

STRATEGIC PRIORITIES

✓ institutional alignment
✓ software sustainability

open calls for eScience domain research

collaborations in advanced eScience technologies

workshops & training

community building & networking

netherlands eScience center

Let’s stay in touch

Check for our open calls

🌐 www.eScienceCenter.nl

✉ info@esciencecenter.nl

☎ +31 20 460 4770

Beyond PC

- 'Big data' renders local storage and processing resources inadequate

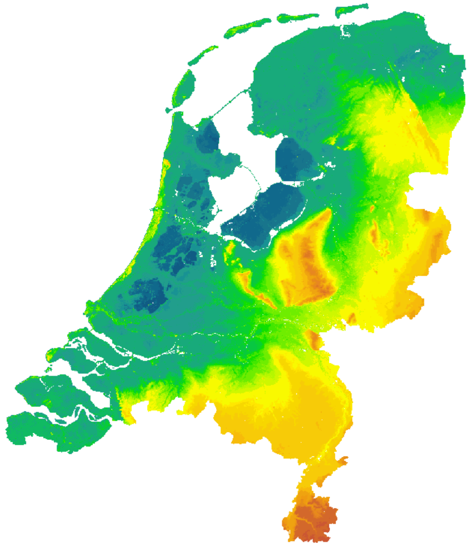
- Resources at larger scale need for processing, analysis and/or further applications (AI)

- Possible providers:
    - (commercial) cloud

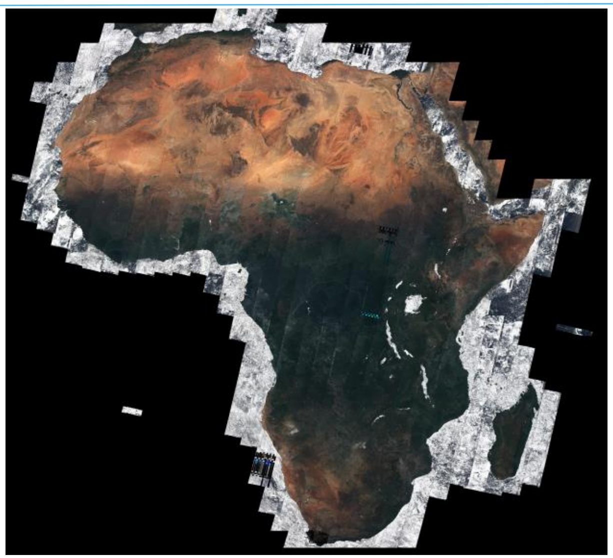
Azure aws

- National/regional/institutional HPC

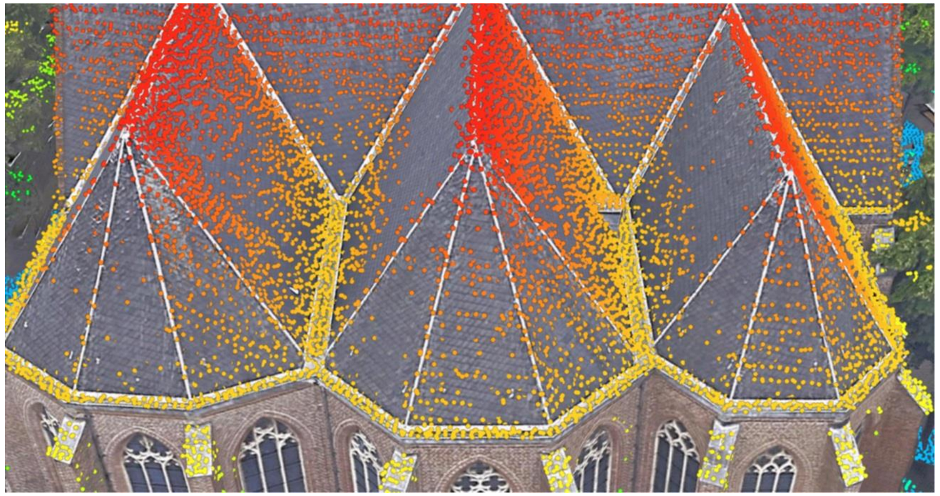
BSC SURF DELFT BLUE



Credit: AHN, Rijkswaterstaat



contains modified Copernicus Sentinel data (2016), processed by Brockmann Consult/ Université catholique de Louvain as part of ESA's Climate Change Initiative Land Cover project, CC BY-SA 3.0 IGO



HPC/HTC vs Cloud

HPC/HTC

➕

- **"No cost", merit based**
- Highly flexible and configurable (Hardware)
- Simple environment customization (and dissemination)
- Well established file system support
- Highly optimized I/O infrastructure
- High level of support
- Compatible with Open Science paradigm and reproducibility requirements

➖

- One-off data retrieval required
- Storage can be problematic (not so for SURF)
- No/limited convenience functions
- Delay between first request and access to resources

Cloud

➕

- No/little need to download data
- Easy configuration via (VM) presets
- Available on demand at requested level
- Possibly available high-level convenience functions (e.g. mosaicing)
- Professional support (if paid for)

➖

- Commerical provider; paid access
- Limited access (on free research allotments)
- Limited flexibility (presets) or intricate config for non-standard requirements
- Support (only) at cost
- Scaling can lead to high costs

Goals for today

- Tools for scaling (geo-spatial) 'big data' workflows
- Easy-to-use framework deployment on HPC/HTC

SURF

SURF presentation (~10-15 min)

SURF services, specifically SPIDER

Pre-start check-in day 3

GO TO

menti.com

ENTER THE CODE

35 35 67 6

0

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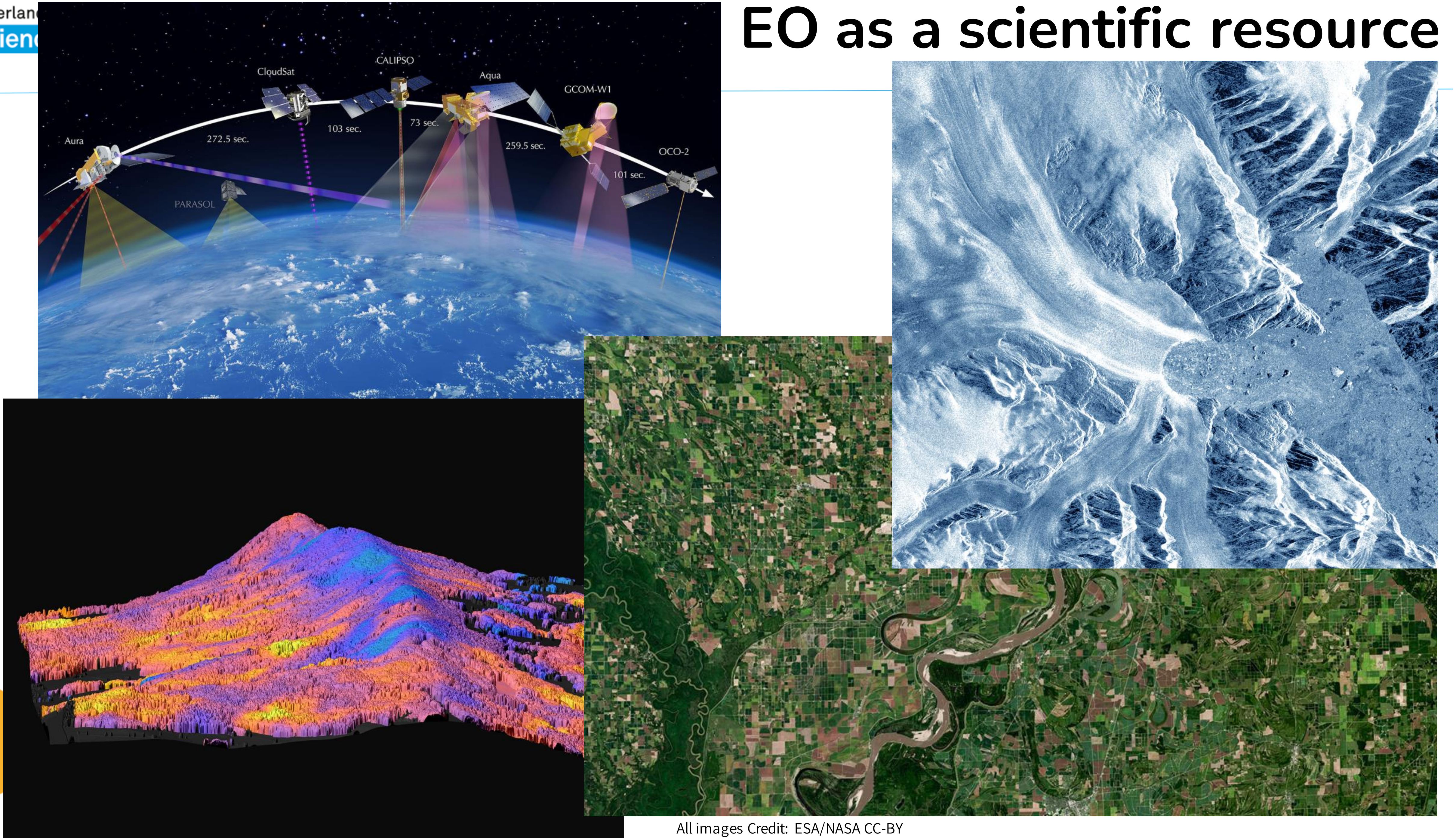
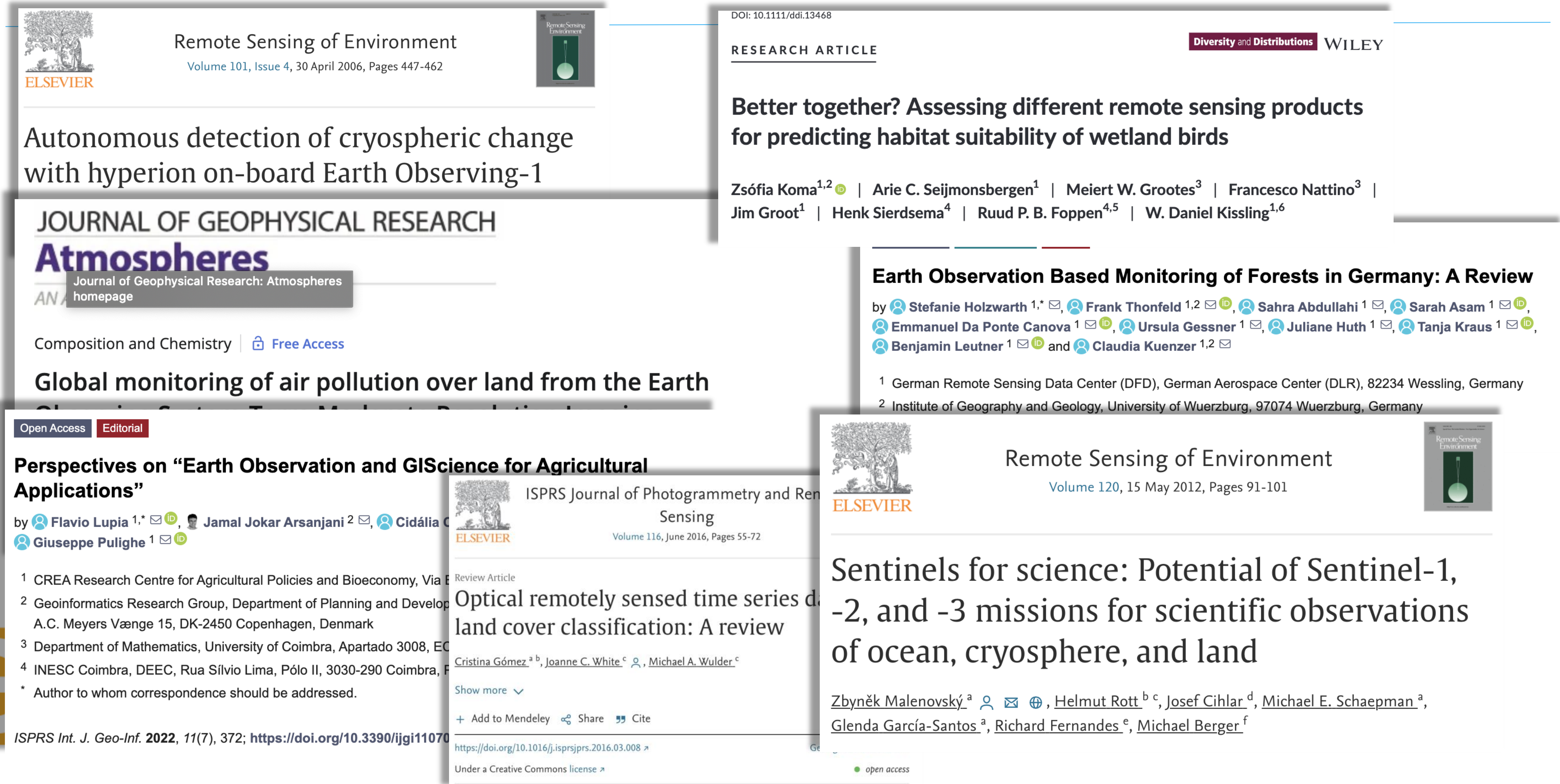
SURF

EO as a scientific resource



All images Credit: ESA/NASA CC-BY

EO as a scientific resource



ELSEVIER

Remote Sensing of Environment

Volume 101, Issue 4, 30 April 2006, Pages 447-462

Autonomous detection of cryospheric change with hyperion on-board Earth Observing-1

JOURNAL OF GEOPHYSICAL RESEARCH

Atmospheres

AN A

Journal of Geophysical Research: Atmospheres homepage

Composition and Chemistry | Free Access

Global monitoring of air pollution over land from the Earth

DOI: 10.1111/ddi.13468

RESEARCH ARTICLE

Diversity and Distributions WILEY

Better together? Assessing different remote sensing products for predicting habitat suitability of wetland birds

Zsófia Koma[1,2] | Arie C. Seijmonsbergen[1] | Meiert W. Grootes[3] | Francesco Nattino[3] | Jim Groot[1] | Henk Sierdsema[4] | Ruud P. B. Foppen[4,5] | W. Daniel Kissling[1,6]

Earth Observation Based Monitoring of Forests in Germany: A Review

by Stefanie Holzwarth [1,*], Frank Thonfeld [1,2], Sahra Abdullahi [1], Sarah Asam [1], Emmanuel Da Ponte Canova [1], Ursula Gessner [1], Juliane Huth [1], Tanja Kraus [1], Benjamin Leutner [1] and Claudia Kuenzer [1,2]

[1] German Remote Sensing Data Center (DFD), German Aerospace Center (DLR), 82234 Wessling, Germany

[2] Institute of Geography and Geology, University of Wuerzburg, 97074 Wuerzburg, Germany

Open Access Editorial

Perspectives on "Earth Observation and GIScience for Agricultural Applications"

by Flavio Lupia [1,*], Jamal Jokar Arsanjani [2], Cidália C Giuseppe Pulighe [1]

[1] CREA Research Centre for Agricultural Policies and Bioeconomy, Via

[2] Geoinformatics Research Group, Department of Planning and Develop A.C. Meyers Vænge 15, DK-2450 Copenhagen, Denmark

[3] Department of Mathematics, University of Coimbra, Apartado 3008, EC

[4] INESC Coimbra, DEEC, Rua Sílvio Lima, Pólo II, 3030-290 Coimbra, F

[*] Author to whom correspondence should be addressed.

ISPRS Int. J. Geo-Inf. **2022**, *11*(7), 372; https://doi.org/10.3390/ijgi11070

ELSEVIER

ISPRS Journal of Photogrammetry and Ren Sensing

Volume 116, June 2016, Pages 55-72

Review Article

Optical remotely sensed time series d land cover classification: A review

Cristina Gómez [a b], Joanne C. White [c], Michael A. Wulder [c]

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https://doi.org/10.1016/j.isprsjprs.2016.03.008

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ELSEVIER

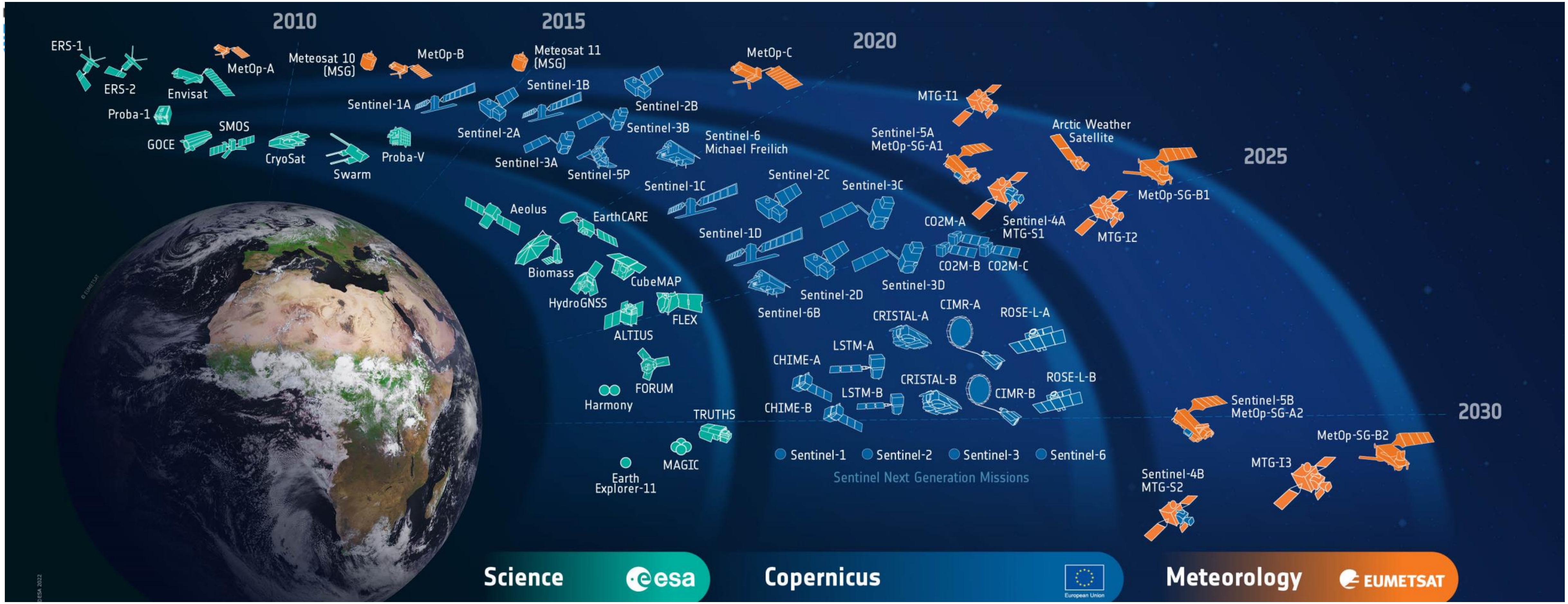
Remote Sensing of Environment

Volume 120, 15 May 2012, Pages 91-101

Sentinels for science: Potential of Sentinel-1, -2, and -3 missions for scientific observations of ocean, cryosphere, and land

Zbyněk Malenovský [a], Helmut Rott [b c], Josef Cihlar [d], Michael E. Schaepman [a], Glenda García-Santos [a], Richard Fernandes [e], Michael Berger [f]

● open access

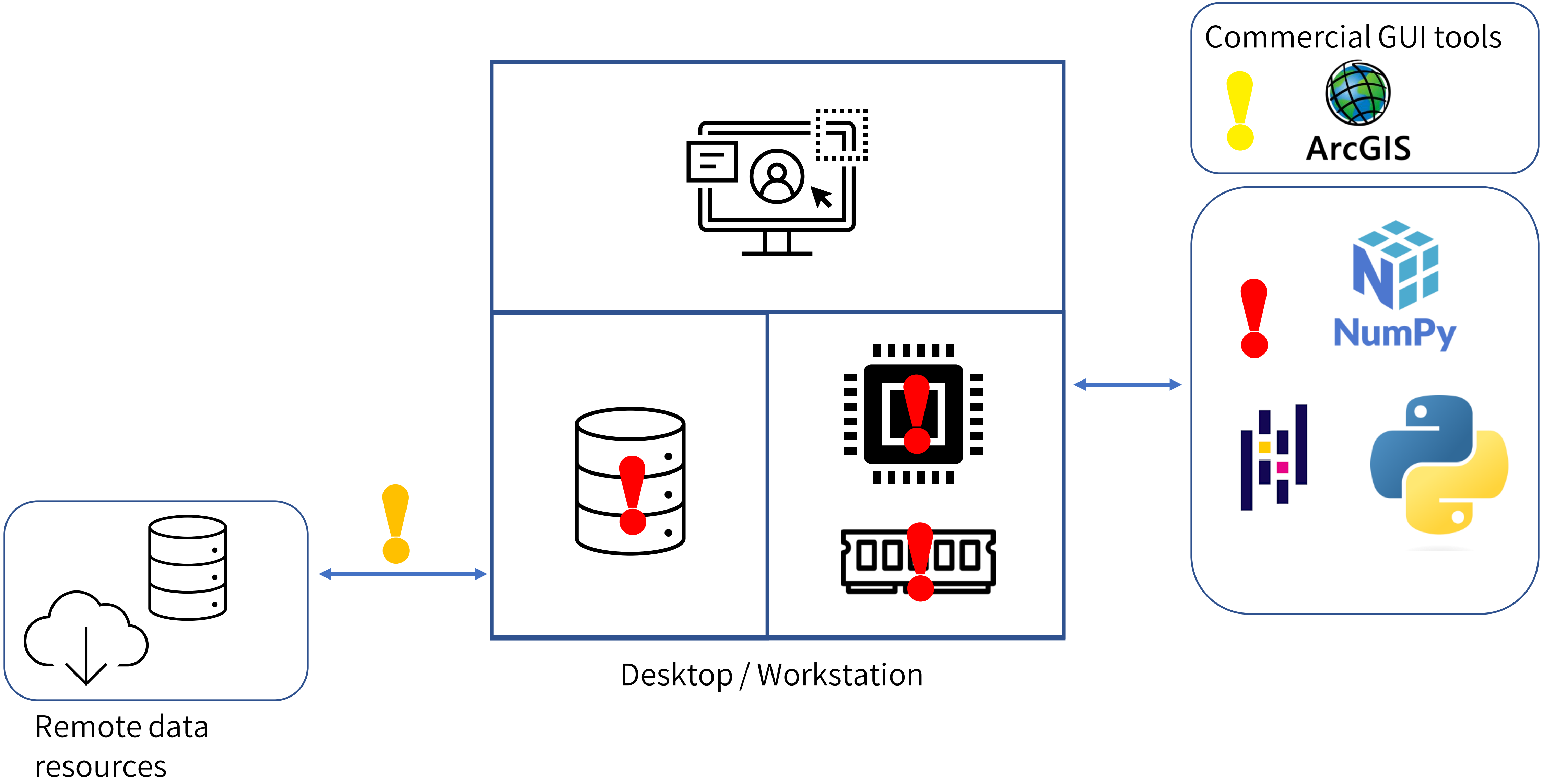


Credit: ESA

The challenge of Big GeoData

- Petabyte scale, high-resolution data - unique opportunity for scientific exploitation
- Fundamental challenge due to volume – storage & processing
- Established (local) processing solutions do not scale

Failure of the status quo

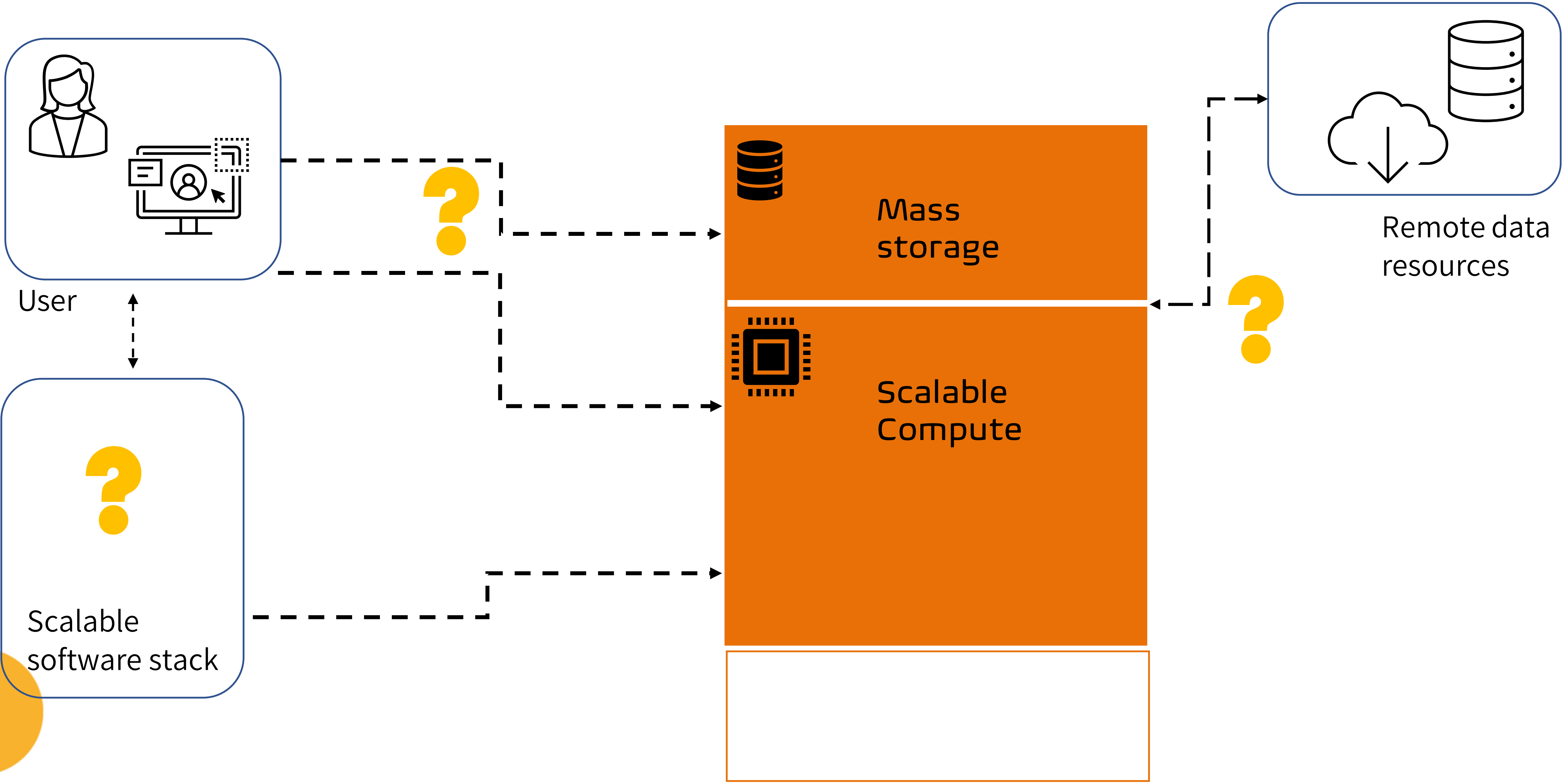


Commercial GUI tools

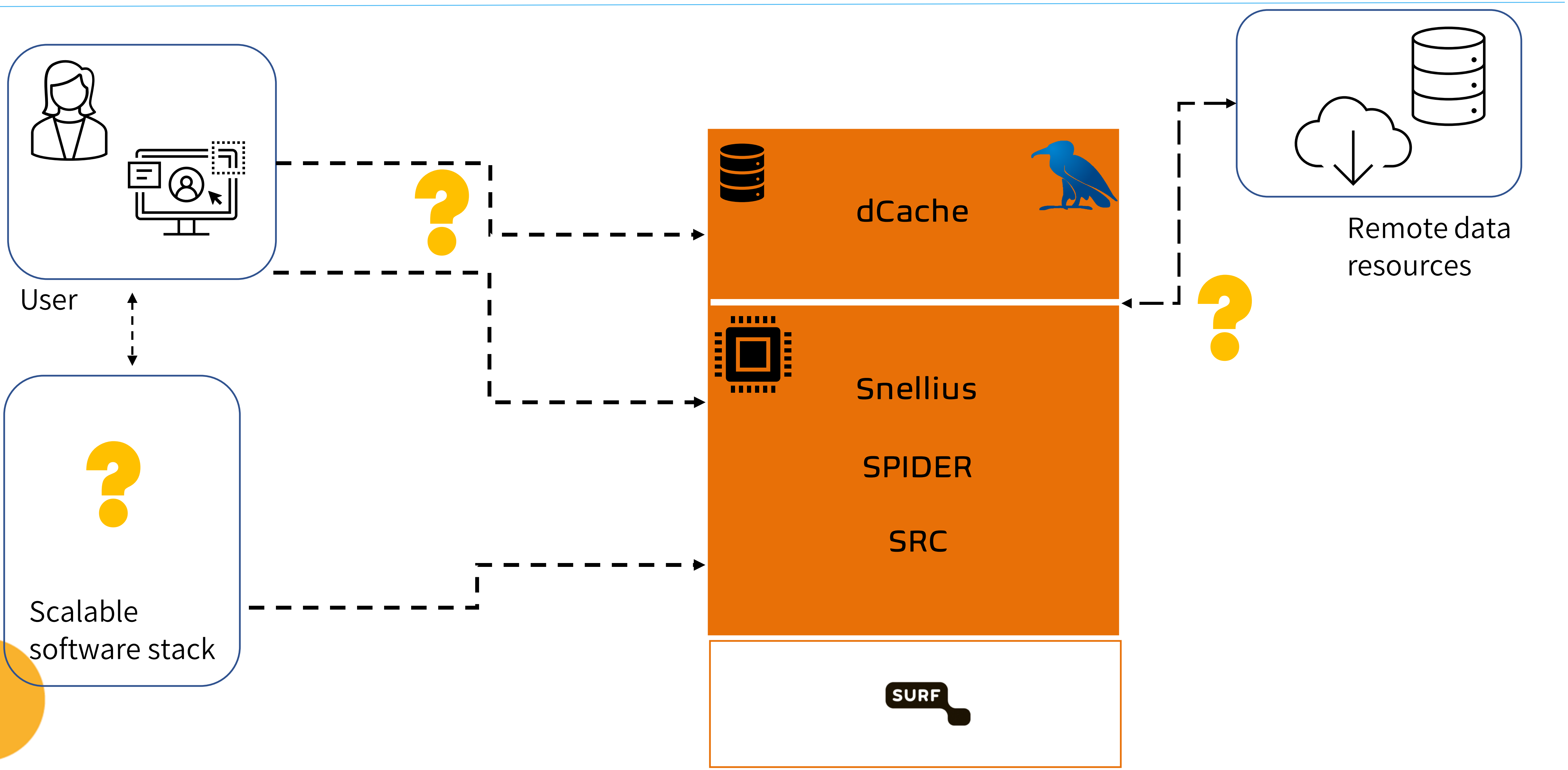
Desktop / Workstation

Remote data resources

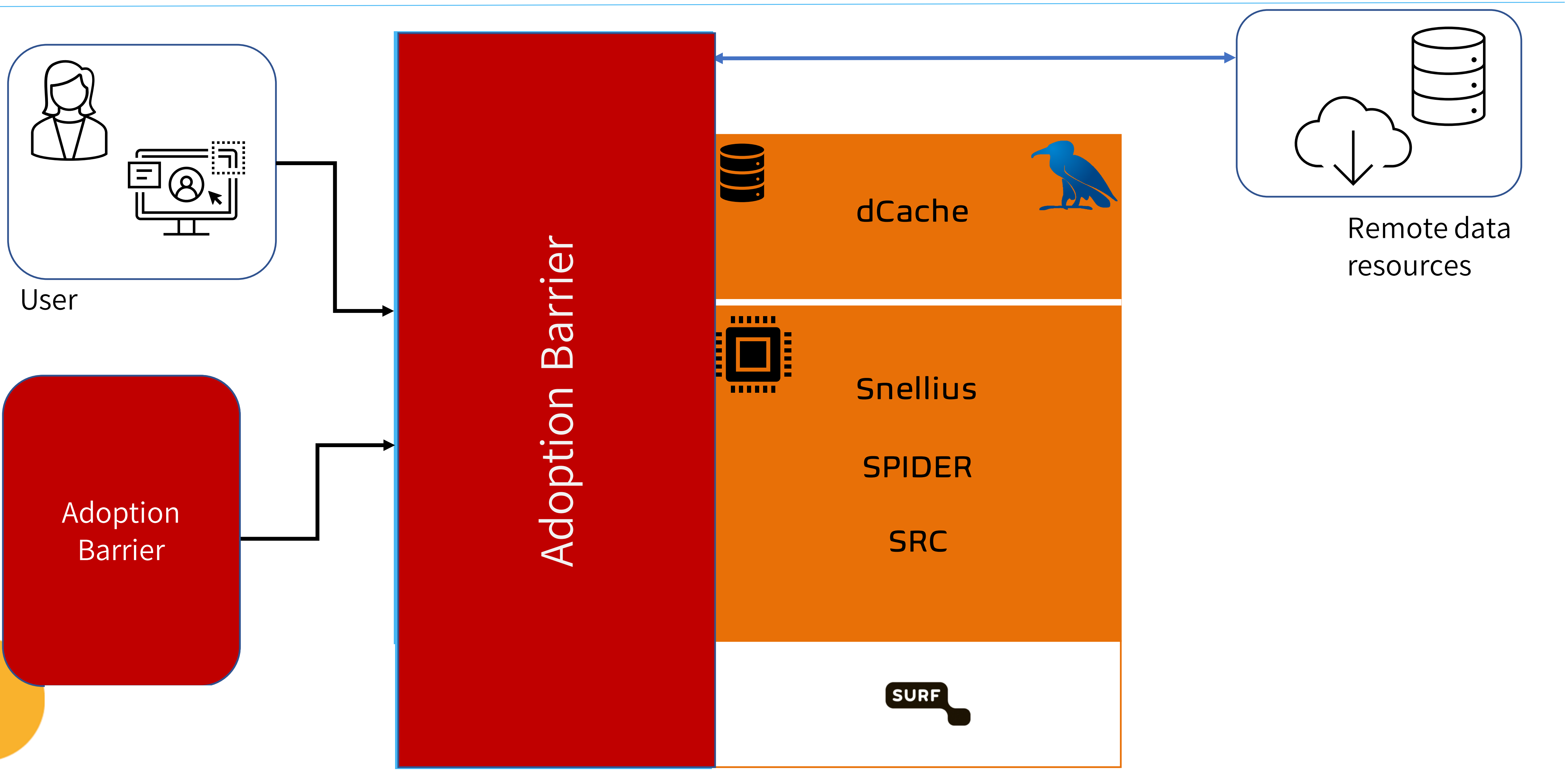
What next?


User
Mass storage
Scalable Compute
Remote data resources
Scalable software stack

What next?


User
Scalable software stack
dCache
Snellius
SPIDER
SRC
SURF
Remote data resources

What is RS-DAT ?



The PANGEO community

Pangeo is first and foremost a community of people working collaboratively to develop software and infrastructure to enable Big Data geoscience research.

Some of the products produced by this community include interconnected software package and deployments of this software in cloud and high-performance-computing environments. Such a deployment is sometimes referred to as a *Pangeo Environment*.

PANGEO

A community platform for Big Data geoscience

Core:
Interoperable, scalable, Python data science stack with geospatial focus

dask

Scalable computation

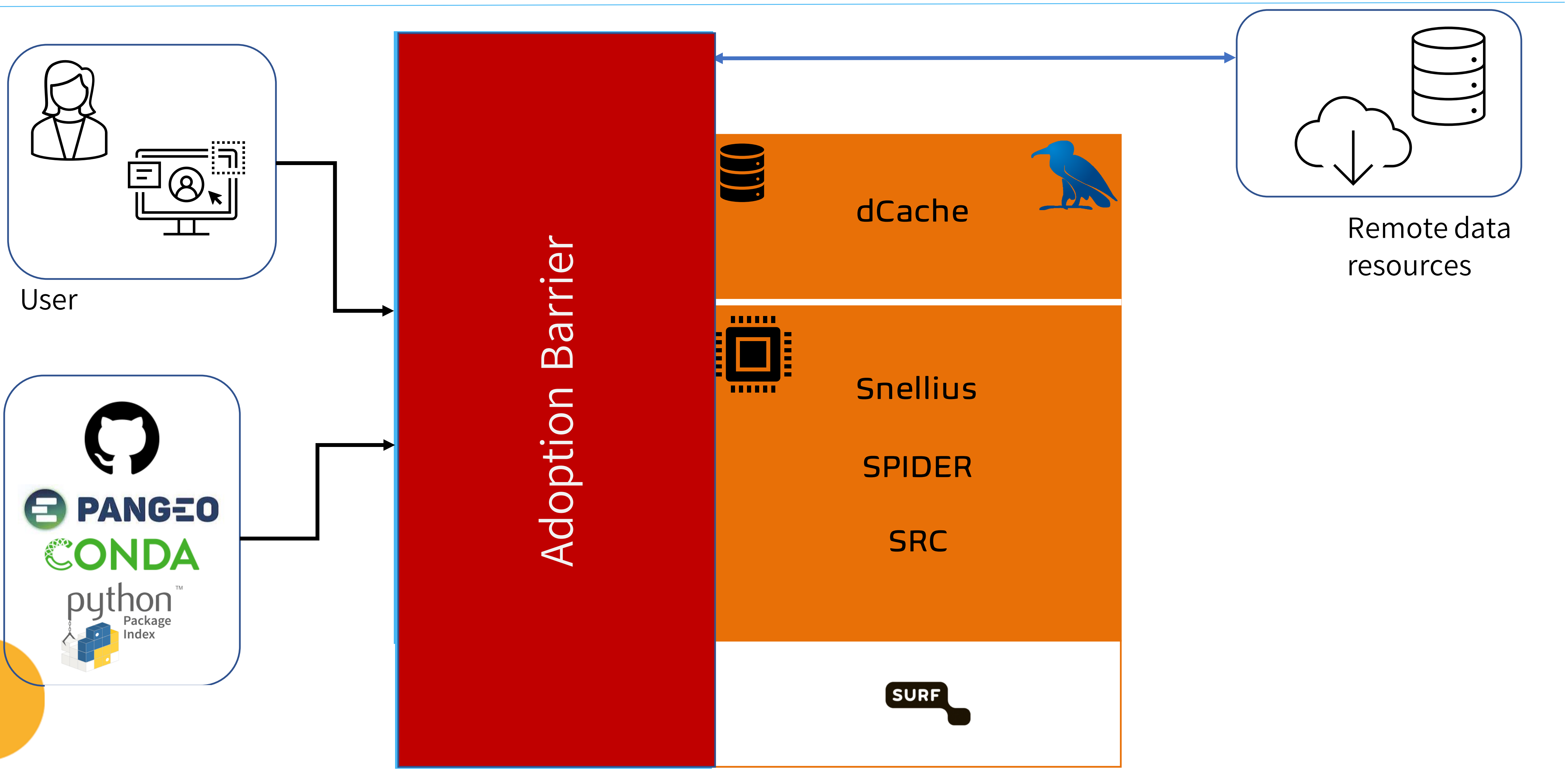
xarray

Rich data model w/ out-of-core support

jupyter

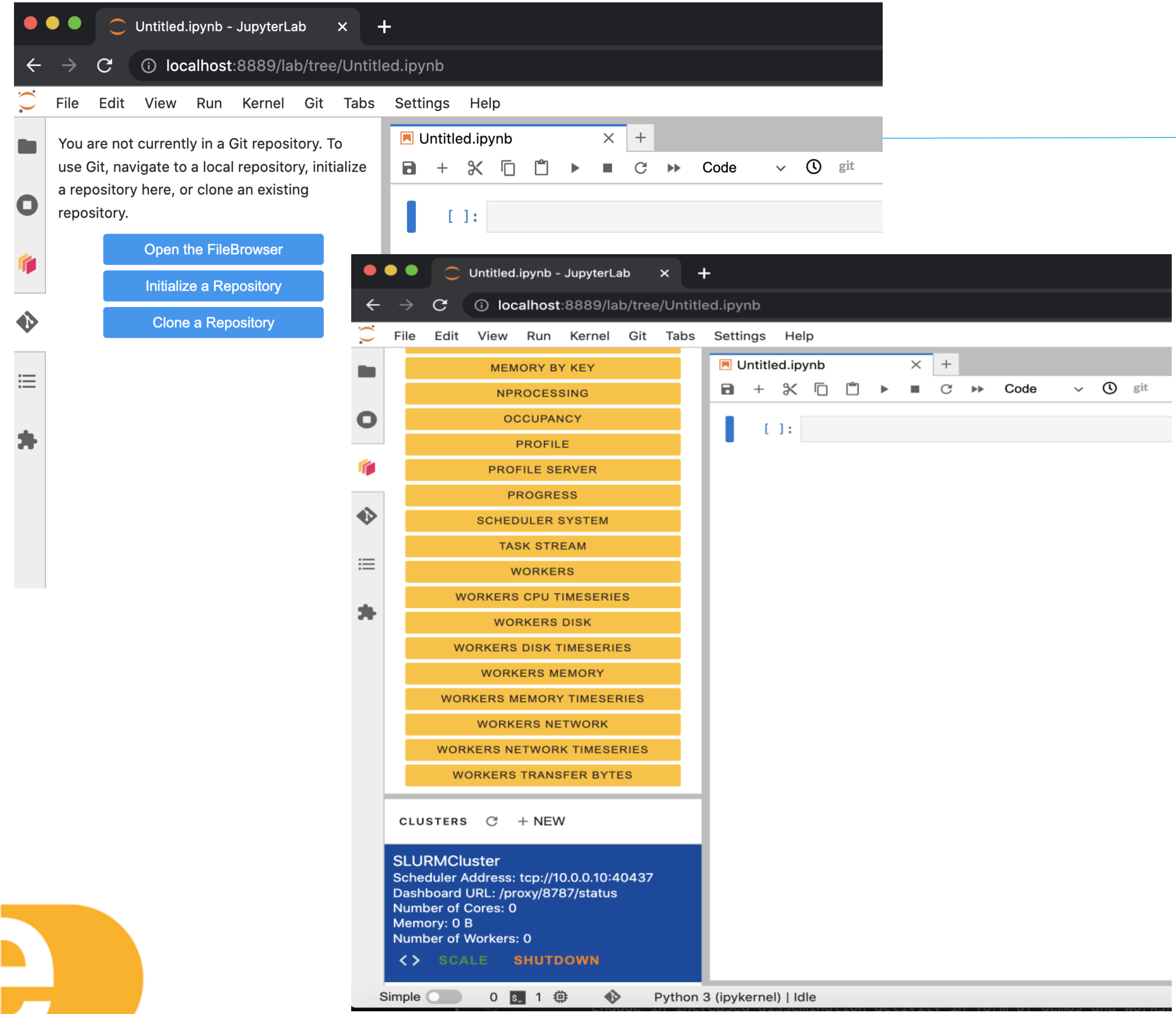
Interactive analysis and execution

What is RS-DAT ?



RS-DAT core in brief

Jupyter at scale



You are not currently in a Git repository. To use Git, navigate to a local repository, initialize a repository here, or clone an existing repository.

SLURMCluster
Scheduler Address: tcp://10.0.0.10:40437
Dashboard URL: /proxy/8787/status
Number of Cores: 0
Memory: 0 B
Number of Workers: 0

- Scale analysis: accustomed interactive workflows, but backed by HPC/Cloud
- Combine Jupyter server with Dask cluster on HPC/HTC/Cluster/Cloud sys tem

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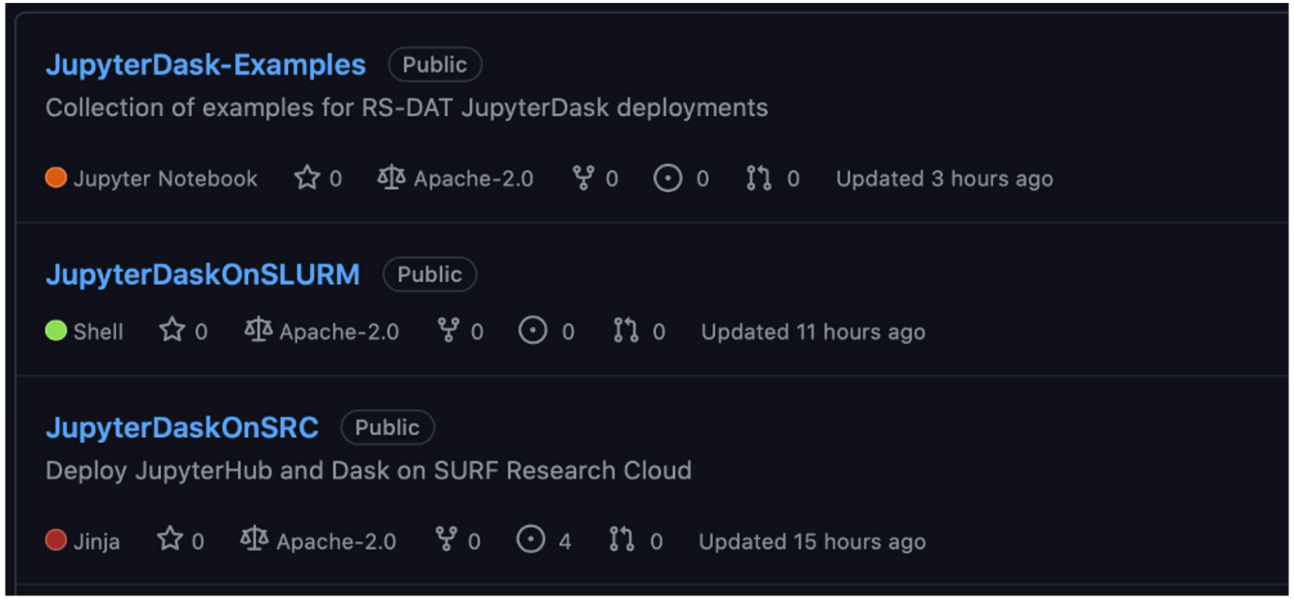
RS-DAT Features

https://github.com/RS-DAT/JupyterDaskOnSLURM



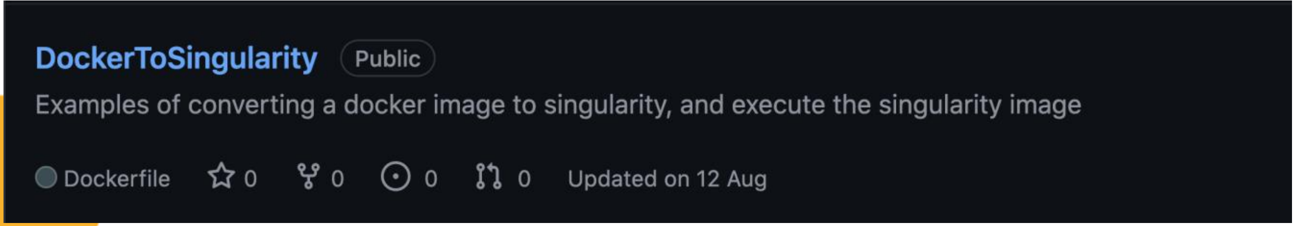
JupyterDask-Examples Public
Collection of examples for RS-DAT JupyterDask deployments
● Jupyter Notebook ☆ 0 ⚖ Apache-2.0 ⑂ 0 ⊙ 0 ⇅ 0 Updated 3 hours ago

JupyterDaskOnSLURM Public
● Shell ☆ 0 ⚖ Apache-2.0 ⑂ 0 ⊙ 0 ⇅ 0 Updated 11 hours ago

JupyterDaskOnSRC Public
Deploy JupyterHub and Dask on SURF Research Cloud
● Jinja ☆ 0 ⚖ Apache-2.0 ⑂ 0 ⊙ 4 ⇅ 0 Updated 15 hours ago

Scalable analysis with Jupyter

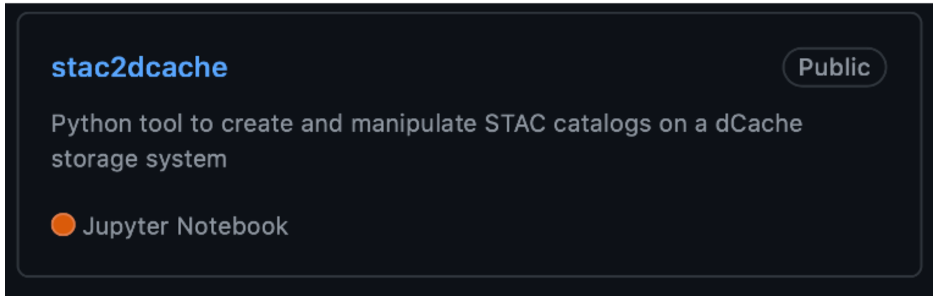
Using legacy (Docker) containers for HPC



DockerToSingularity Public
Examples of converting a docker image to singularity, and execute the singularity image
● Dockerfile ☆ 0 ⑂ 0 ⊙ 0 ⇅ 0 Updated on 12 Aug

https://github.com/RS-DAT/DockerToSingularity

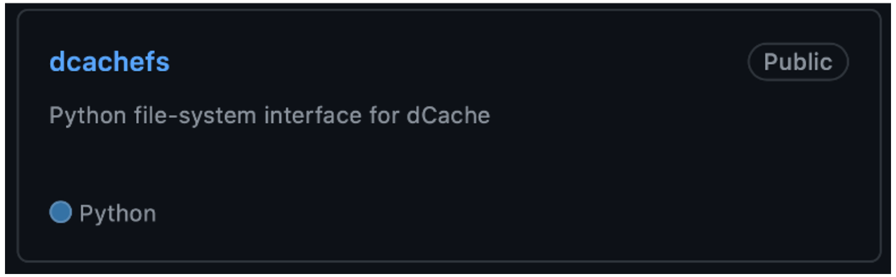
https://github.com/NLeSC-GO-common-infrastructure/stac2dcache



stac2dcache Public
Python tool to create and manipulate STAC catalogs on a dCache storage system
● Jupyter Notebook

utility functions to manage STAC catalogs (and the underlying data) on dCache.

https://github.com/NLeSC-GO-common-infrastructure/dcachefs

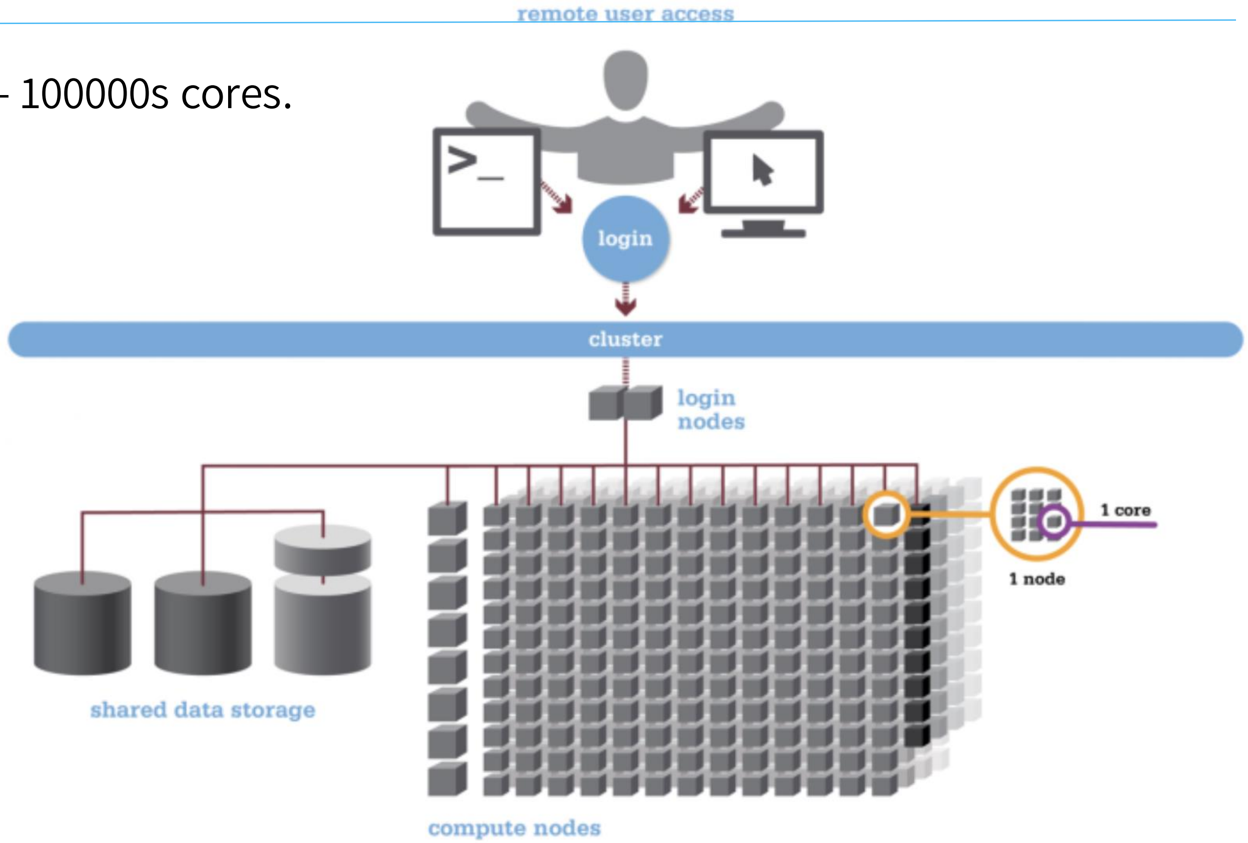


dcachefs Public
Python file-system interface for dCache
● Python

Python interface to dCache

HPC/HTC basics

- Clusters of compute servers (100s –1000s nodes), with 10000s – 100000s cores.
- High bandwidth internal network between nodes
- Shared RAM per node; configurable
- Shared storage/mounted FS
- Generally Linux based (command line, SSH keys)



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- High bandwidth internal network between nodes
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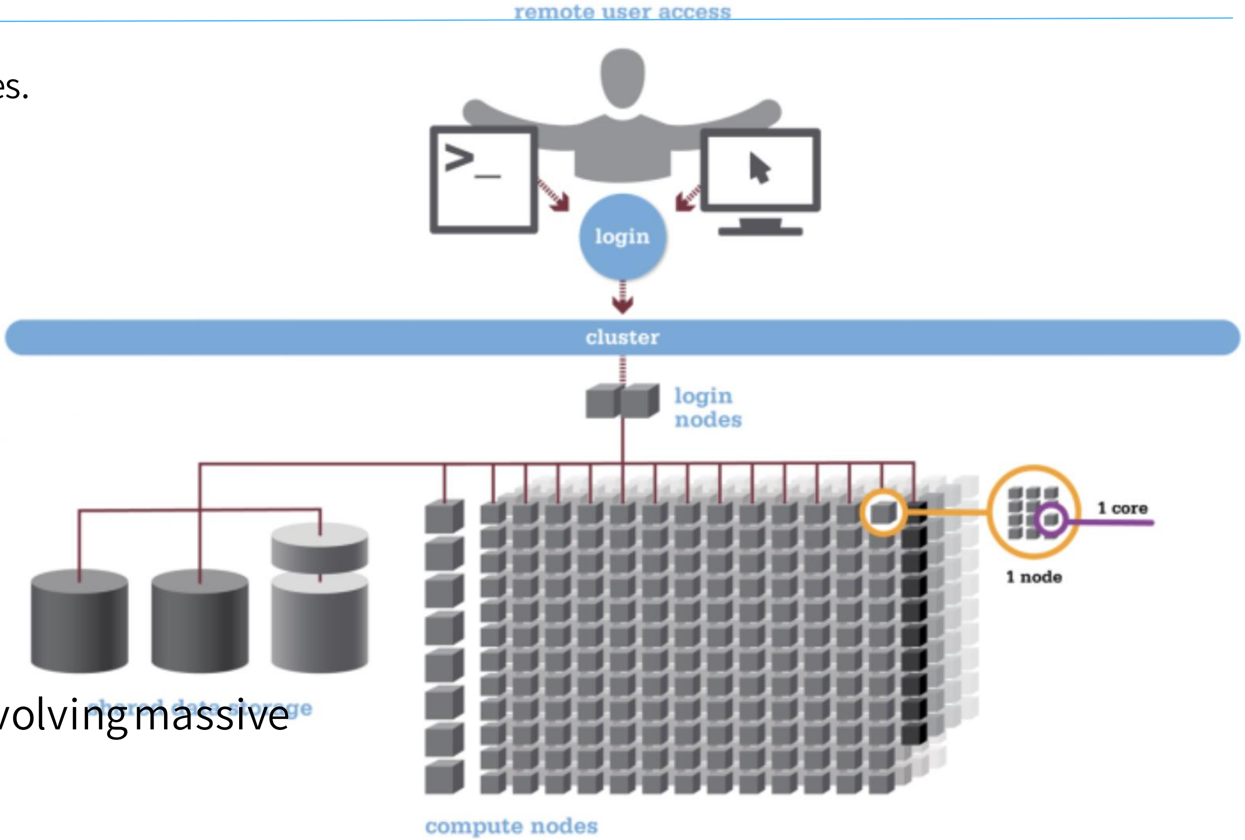
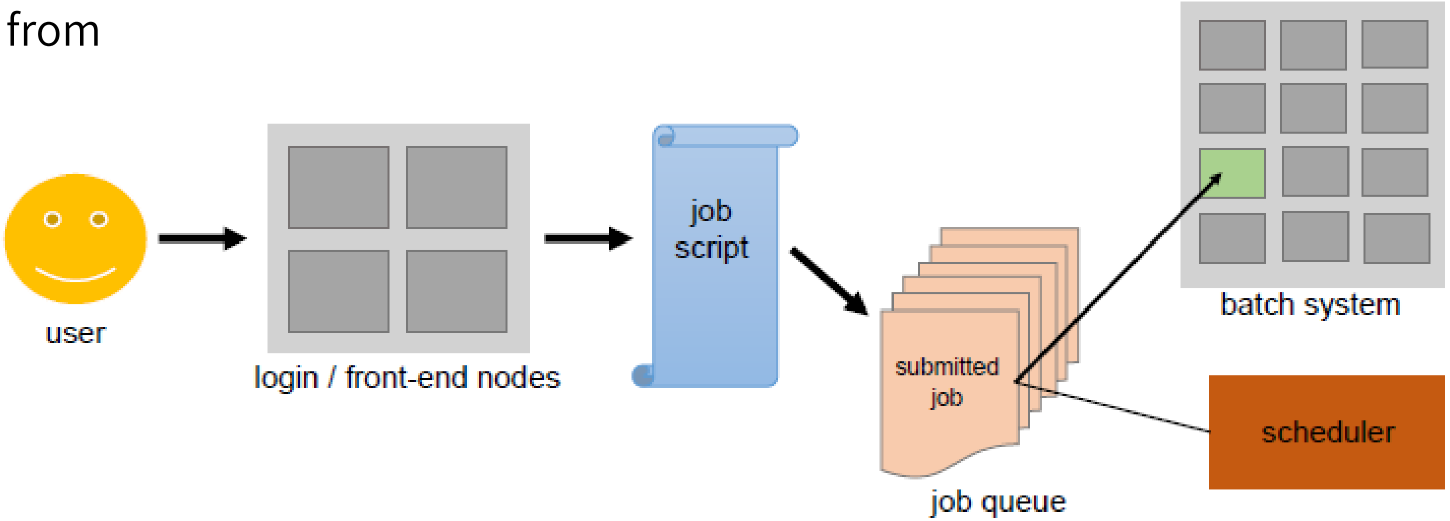
- Shared storage/mounted FS
- Generally Linux based (command line, SSH keys)

- **Designed for non-interactive, large jobs or batch jobs**
- Either VERY computationally expensive (classic HPC) and/or involving massive data volumes tto process (HTC)
- **HPC systems are a SHARED resource. (login, etiquette)**
- **Resources must be allocated and jobs scheduled**



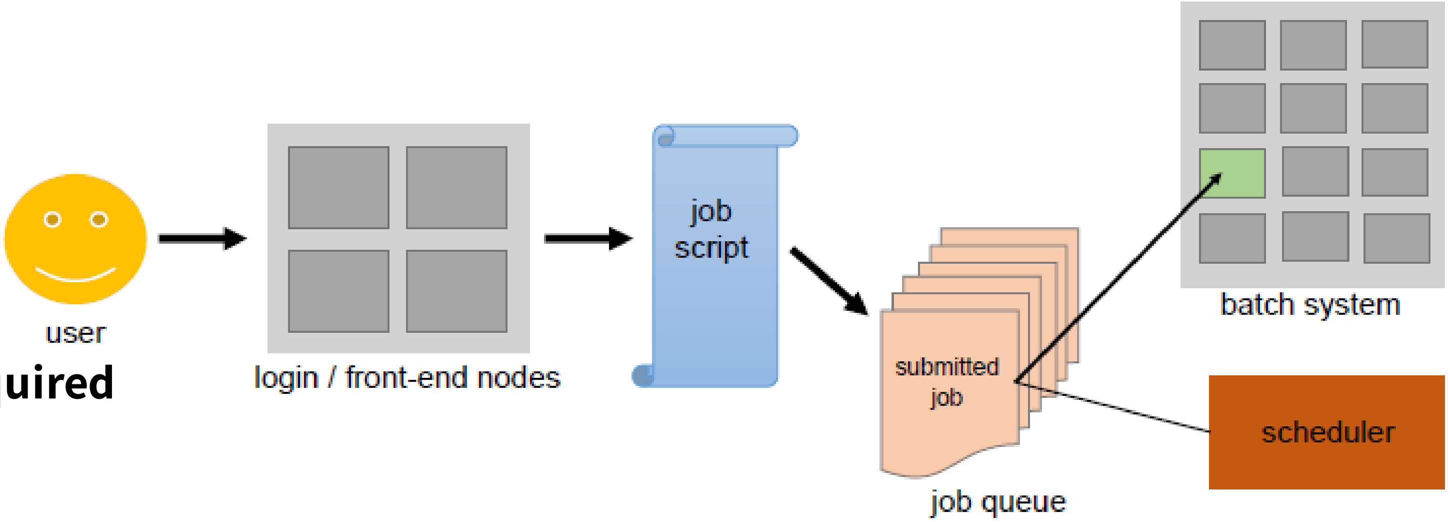
scheduling

- HPC is shared system running multiple jobs from users.
- Need system/software to handle resource allocation
 The batch scheduler



scheduling

- HPC is shared system running multiple jobs from users.
- Need system/software to handle resource allocation
  The batch scheduler
- **Elements of scheduling:**
  - **Job script: declaration of job and required resources**
  - **Job queue: ordered registry of submitted job(script)s**
  - **Scheduler: Software running scheduling algorithm over job queue and allocating resources and priority**



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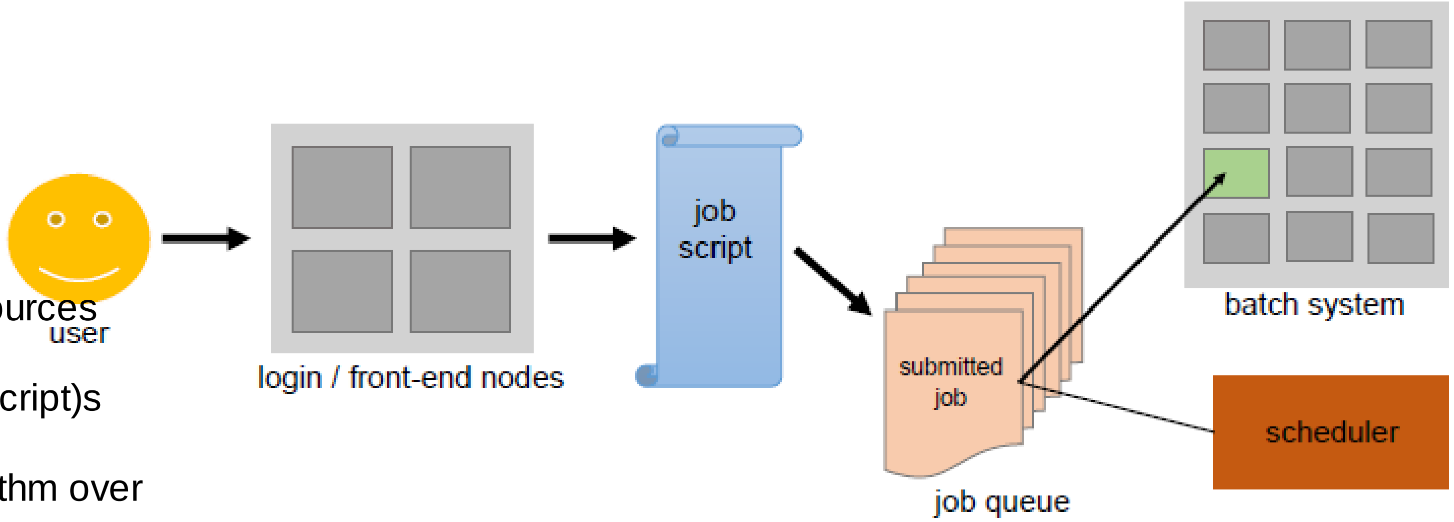

- **Scheduling algorithms:**
  - First come, first served
    Everything scheduled, but inefficient
  - Shortest job first
    Long/resource heavy may never be scheduled

scheduling

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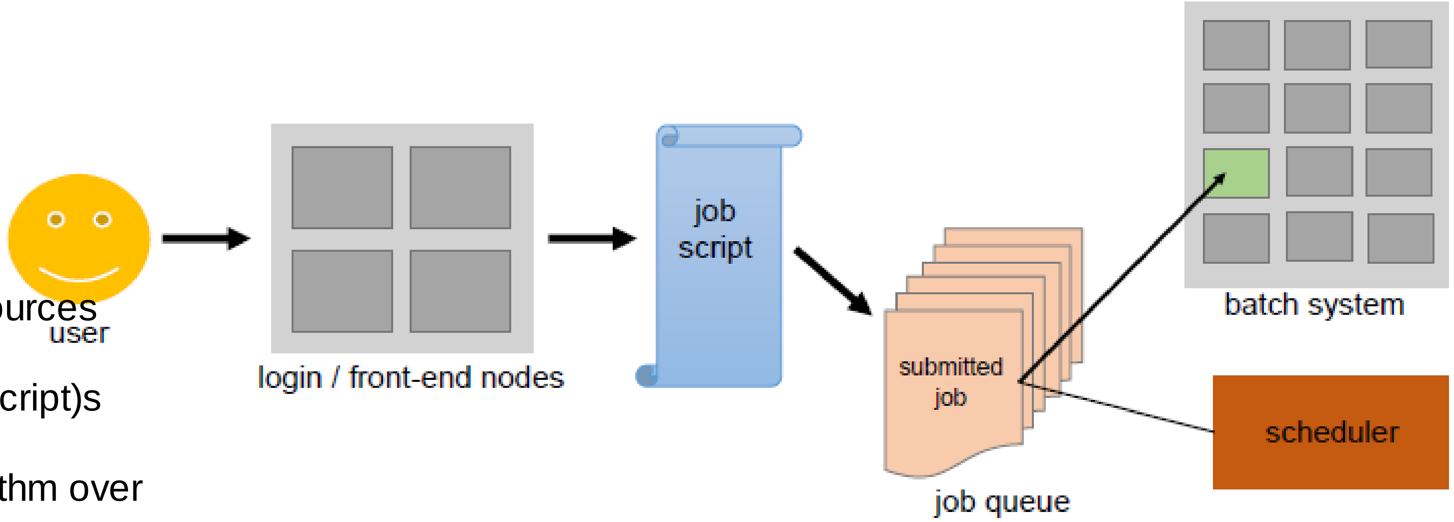
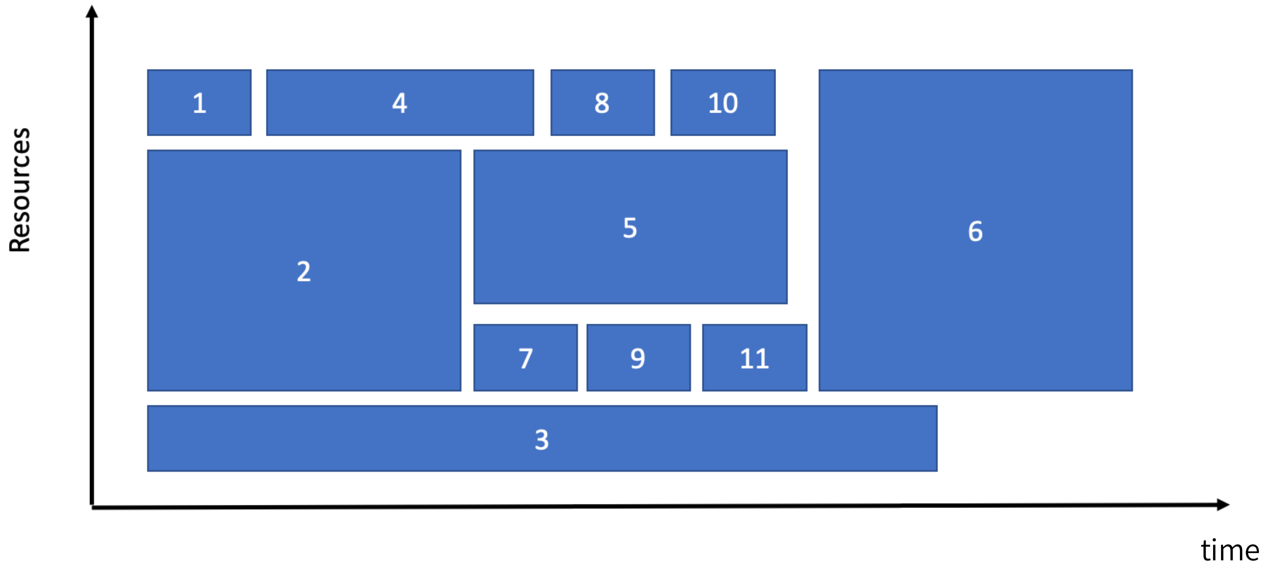


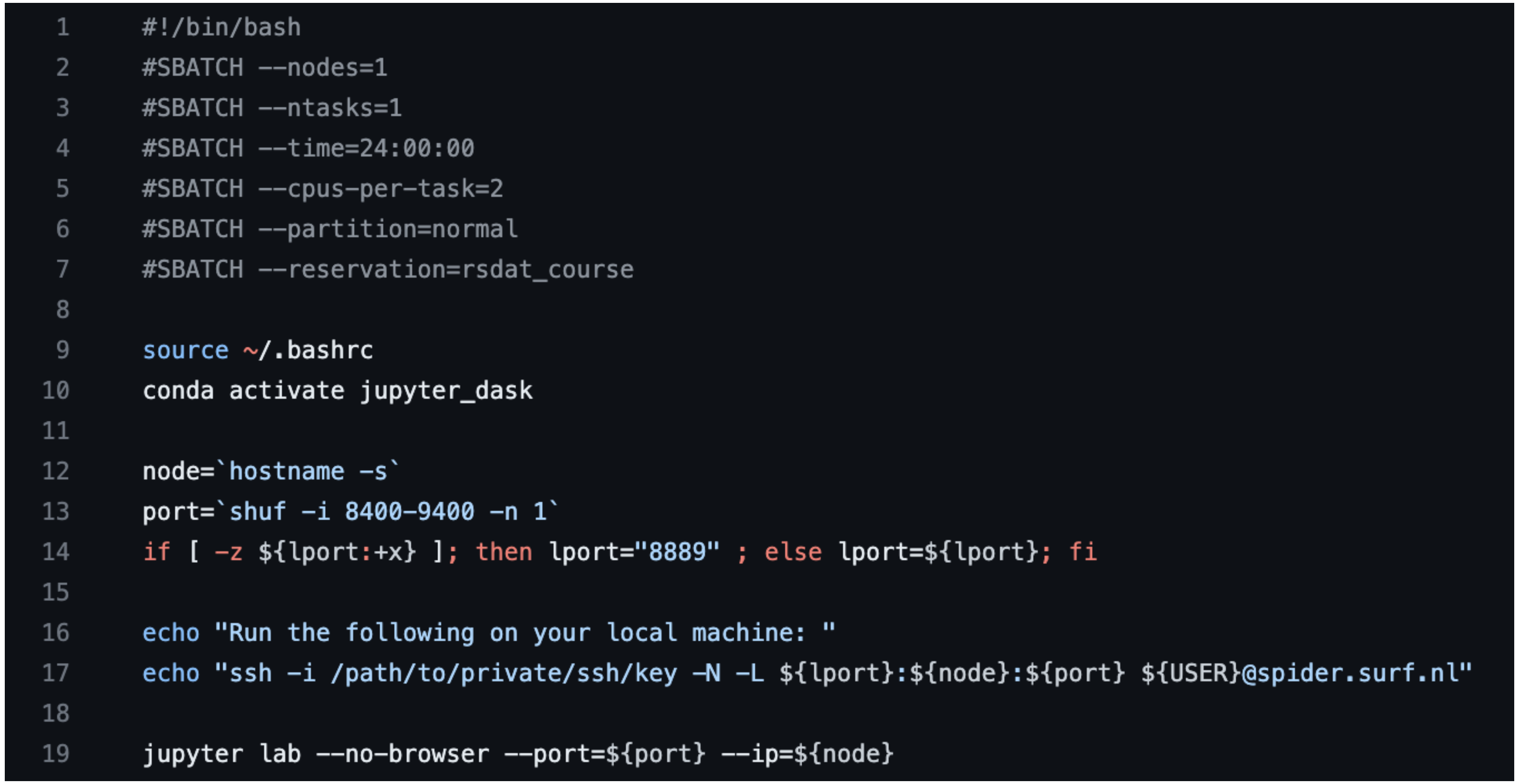
- **Scheduling algorithms:**
  - First come, first served
    Everything scheduled, but inefficient, long wait
  - Shortest job first
    Long/resource heavy may never be scheduled
  - Backfilling
    - Combine and interleave, all scheduled



scheduling

- SLURM scheduler on SURF systems (Spider, Snellius)

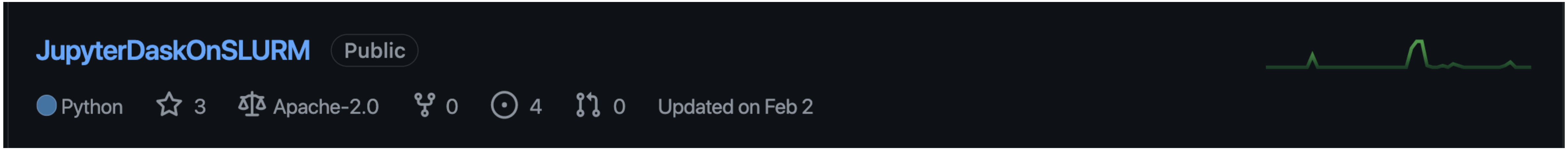
- SLURM at a glance https://slurm.schedmd.com/quickstart.html



```bash
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --time=24:00:00
#SBATCH --cpus-per-task=2
#SBATCH --partition=normal
#SBATCH --reservation=rsdat_course

source ~/.bashrc
conda activate jupyter_dask

node=`hostname -s`
port=`shuf -i 8400-9400 -n 1`
if [ -z ${lport:+x} ]; then lport="8889" ; else lport=${lport}; fi

echo "Run the following on your local machine: "
echo "ssh -i /path/to/private/ssh/key -N -L ${lport}:${node}:${port} ${USER}@spider.surf.nl"

jupyter lab --no-browser --port=${port} --ip=${node}
```

Jupyter Dask on Slurm

SURF H*C Infrastructure: Spider (HTC), Snellius (HPC); SLURM scheduler



JupyterDaskOnSLURM Public

Python ☆ 3 Apache-2.0 0 4 0 Updated on Feb 2

- JupyterLab instance with Dask and Git extensions, scalable Dask cluster, running on SLURM managed HTC/HPC system
- Basic idea
  - Launch JupyterLab server and Dask scheduler as long-running batch job
  - SSH port-forwarding to connect to JupyterLab server
  - Launch workers as short-lived batch jobs (fast thru queue)