

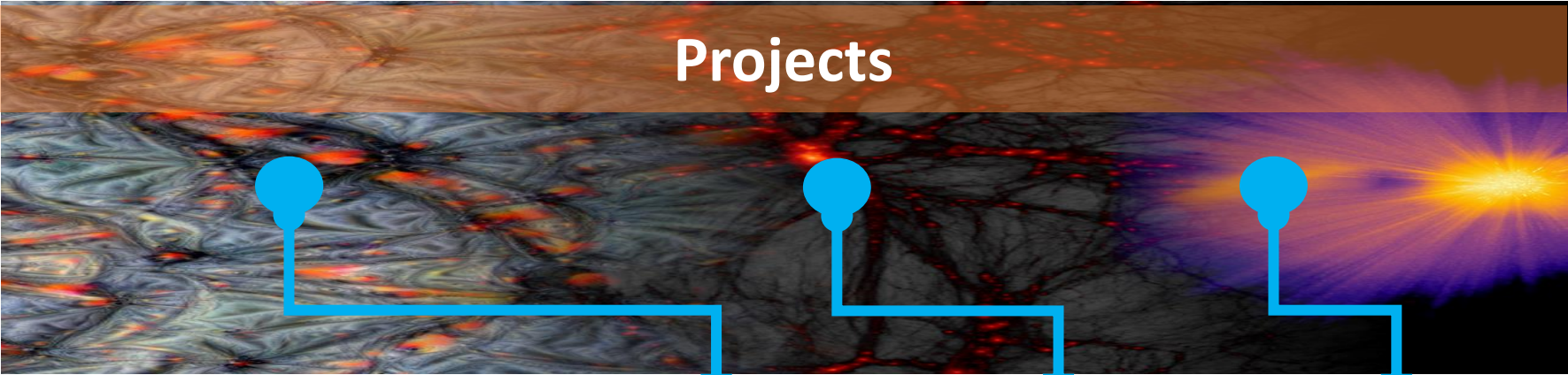


Leibniz-Institut für
Astrophysik Potsdam

Optimizing Scientific Workflows

Integrating REANA with PUNCH Infrastructure

Research interests



HPC
BigDATA
ML
MPI
OpenMPI
Visualisation

HESTIA:
High-resolution
Environmental
Simulations of The
Immediate Area

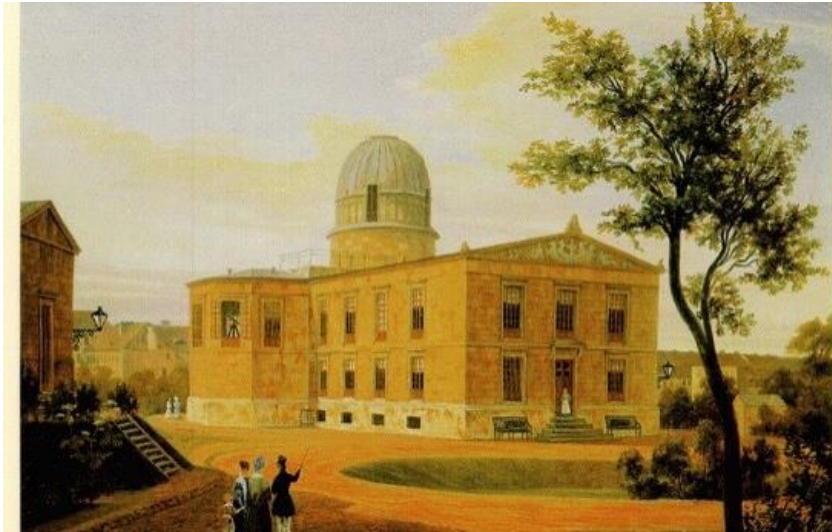
StarHorse:
Photo-astrometric
distances,
extinctions, and
astrophysical
parameters for Gaia
stars brighter than $G = 18$

colab.aip.de cloud.aip.de vr.aip.de

Nationale Forschungs-
Daten Infrastruktur [NFDI](http://www.nfdi.de)



From Berlin to Babelsberg



The Berliner Sternwarte in Berlin-Dorotheenstadt, today Berlin-Mitte.



The new Sternwartengebäude in Babelsberg, built 1913.

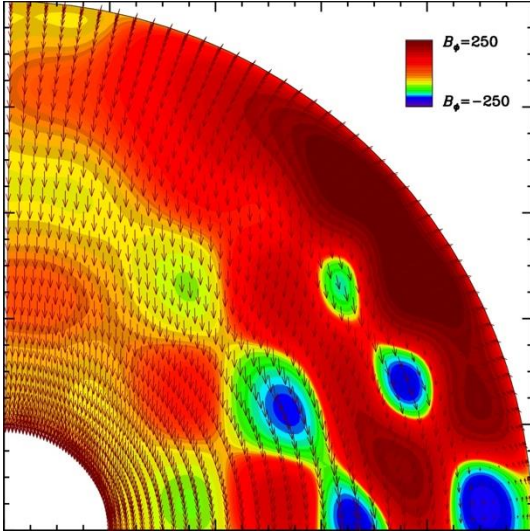
The Berliner Sternwarte, founded in 1700, moved to 1913 Babelsberg because the growing city made scientific observations difficult. Light pollution and vibrations from traffic being the main reasons

Changing Names



From the Zentralinstitut für Astrophysik (1969) after the wall came down the Astrophysikalische Institut Potsdam (1992) was founded. In 2011 ithe AIP was renamed to **Leibniz-Institut für Astrophysik Potsdam (AIP)**, to emphasize the membership with the Leibniz-Gemeinschaft.

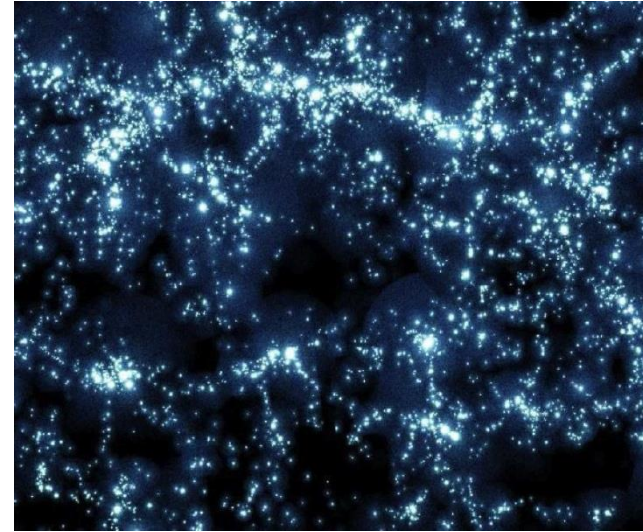
Research Areas



Cosmic Magnetic Fields

Research on solar, stellar and galactic magnetic fields and magnetohydrodynamic (MHD) mechanisms.

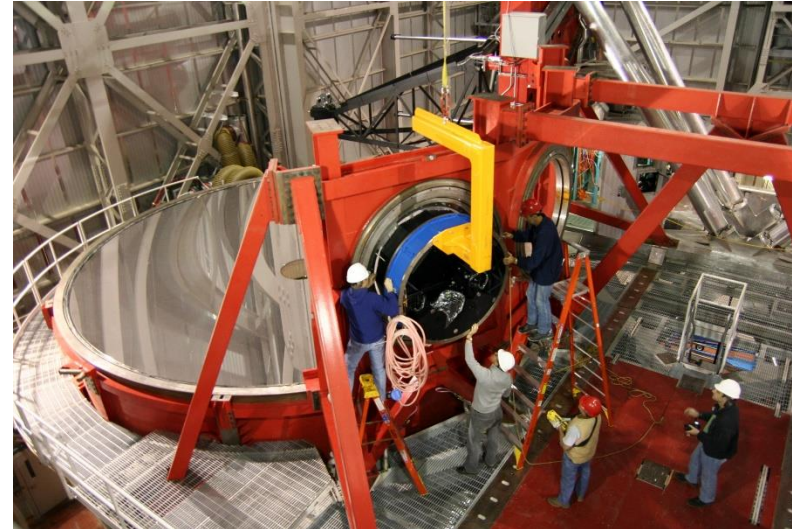
<https://www.aip.de>



Extragalactic Astrophysics

Active galaxies and quasars. Galactic archaeology and extragalactic research based on high resolution simulations.

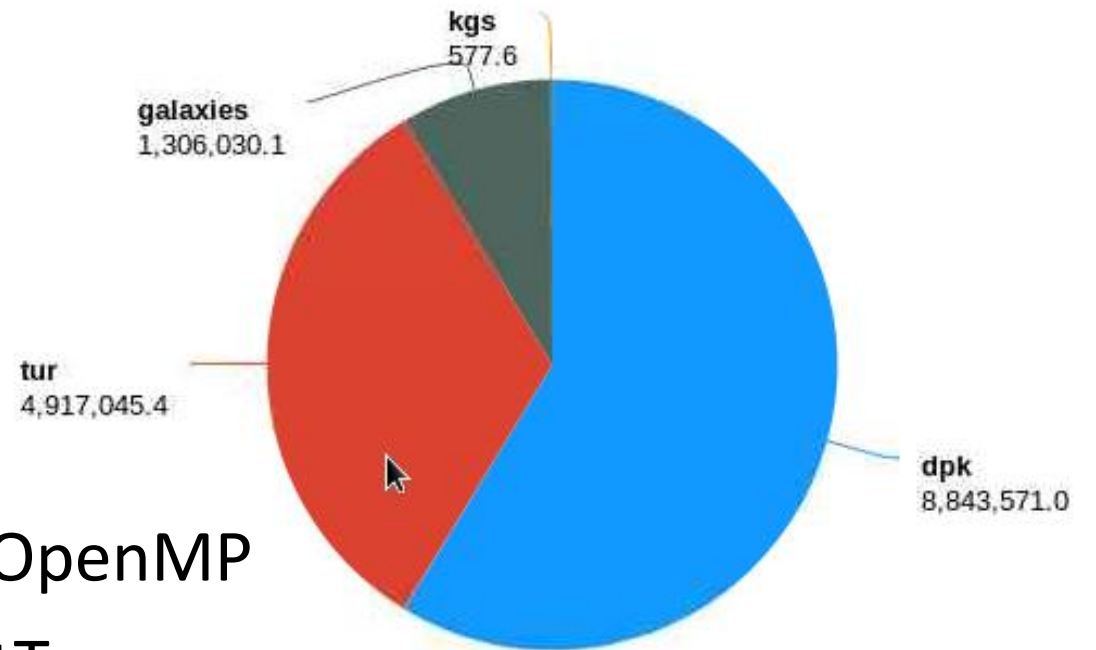
Research technology and infrastructure



„Development of Research technology and infrastructure“ ensures the scientific endeavors of AIP and also its participation in international astronomical projects. AIP has construction workshops and labs for instrumentation, especially with fiber optics, ex: AIP is lead institute of the **4MOST** project a fibre-fed spectroscopic survey facility on the [VISTA telescope](#), op-2021)

Who is using most of the CPU time?

- Cosmology:
 - MHD+Gravity+Gasdynamics
 - Starformation, Cosmic Rays, BH...
 - Magneto-hydrodynamics: MHD
 - Data processing from telescopes
-
- Adaptive unstructured mesh, MPI-OpenMP
 - Magneto-hydrodynamics: AMR-OctTree
 - Data processing from telescopes: python, c, java, other



Languages

AIP/Clusters

- Python
- C/C++
- Fortran
- IDL
- Java
- Perl
- R
- ?Cuda?

Energy Efficiency across Programming Languages How Do Energy, Time, and Memory Relate?

Rui Pereira et al 2017

<https://doi.org/10.1145/3136014.3136031>

Table 4. Normalized global results for Energy, Time, and Memory

Total					
Energy		Time		Mb	
(c) C	1.00	(c) C	1.00	(c) Pascal	1.00
(c) Rust	1.03	(c) Rust	1.04	(c) Go	1.05
(c) C++	1.34	(c) C++	1.56	(c) C	1.17
(c) Ada	1.70	(c) Ada	1.85	(c) Fortran	1.24
(v) Java	1.98	(v) Java	1.89	(c) C++	1.34
(c) Pascal	2.14	(c) Chapel	2.14	(c) Ada	1.47
(c) Chapel	2.18	(c) Go	2.83	(c) Rust	1.54
(v) Lisp	2.27	(c) Pascal	3.02	(v) Lisp	1.92
(c) Ocaml	2.40	(c) Ocaml	3.09	(c) Haskell	2.45
(c) Fortran	2.52	(v) C#	3.14	(i) PHP	2.57
(c) Swift	2.79	(v) Lisp	3.40	(c) Swift	2.71
(c) Haskell	3.10	(c) Haskell	3.55	(i) Python	2.80
(v) C#	3.14	(c) Swift	4.20	(c) Ocaml	2.82
(c) Go	3.23	(c) Fortran	4.20	(v) C#	2.85
(i) Dart	3.83	(v) F#	6.30	(i) Hack	3.34
(v) F#	4.13	(i) JavaScript	6.52	(v) Racket	3.52
(i) JavaScript	4.45	(i) Dart	6.67	(i) Ruby	3.97
(v) Racket	7.91	(v) Racket	11.27	(c) Chapel	4.00
(i) TypeScript	21.50	(i) Hack	26.99	(v) F#	4.25
(i) Hack	24.02	(i) PHP	27.64	(i) JavaScript	4.59
(i) PHP	29.30	(v) Erlang	36.71	(i) TypeScript	4.69
(v) Erlang	42.23	(i) Jruby	43.44	(v) Java	6.01
(i) Lua	45.98	(i) TypeScript	46.20	(i) Perl	6.62
(i) Jruby	46.54	(i) Ruby	59.34	(i) Lua	6.72
(i) Ruby	69.91	(i) Perl	65.79	(v) Erlang	7.20
(i) Python	75.88	(i) Python	71.90	(i) Dart	8.64
(i) Perl	79.58	(i) Lua	82.91	(i) Jruby	19.84

Data Scales

- Cosmological simulations: >5PB(active)
- Observations(preserve/provide service):
 - GAIA: until now about 500TB, serving 200TB (DB) , soon >1PB (+2025)
 - Applaus: 200TB (photo plates archive)
 - 4MOST: GAIA+?
 - Pepsii: 250TB+
 - Stella- robotic telescope: 150TB+
- Data sizes:
 - 1k up to +32GB single files

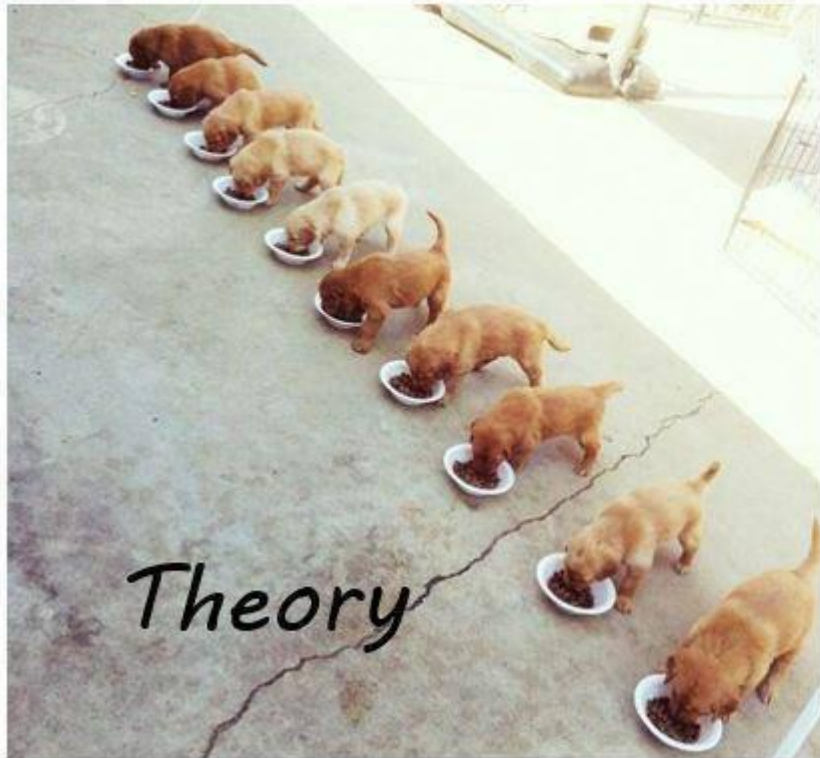
Note:

for **5PB** one need to get also backup:

- 5PB-**300000**€ storage system
- **50000**€ For backup system
- power consumption: 500TB - 0.4kWh, **5y** to keep 5PB up and running is about: **160000**€ for power consumption

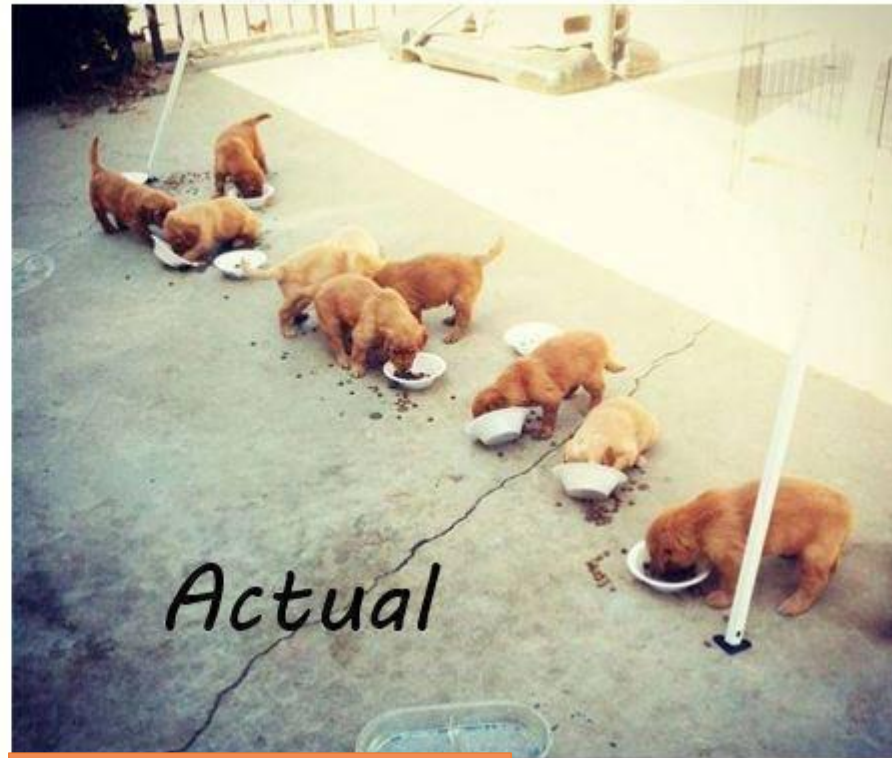
HPC admins: Users software

Multithreaded programming



Theory

Jobqueue



Actual

Interactive

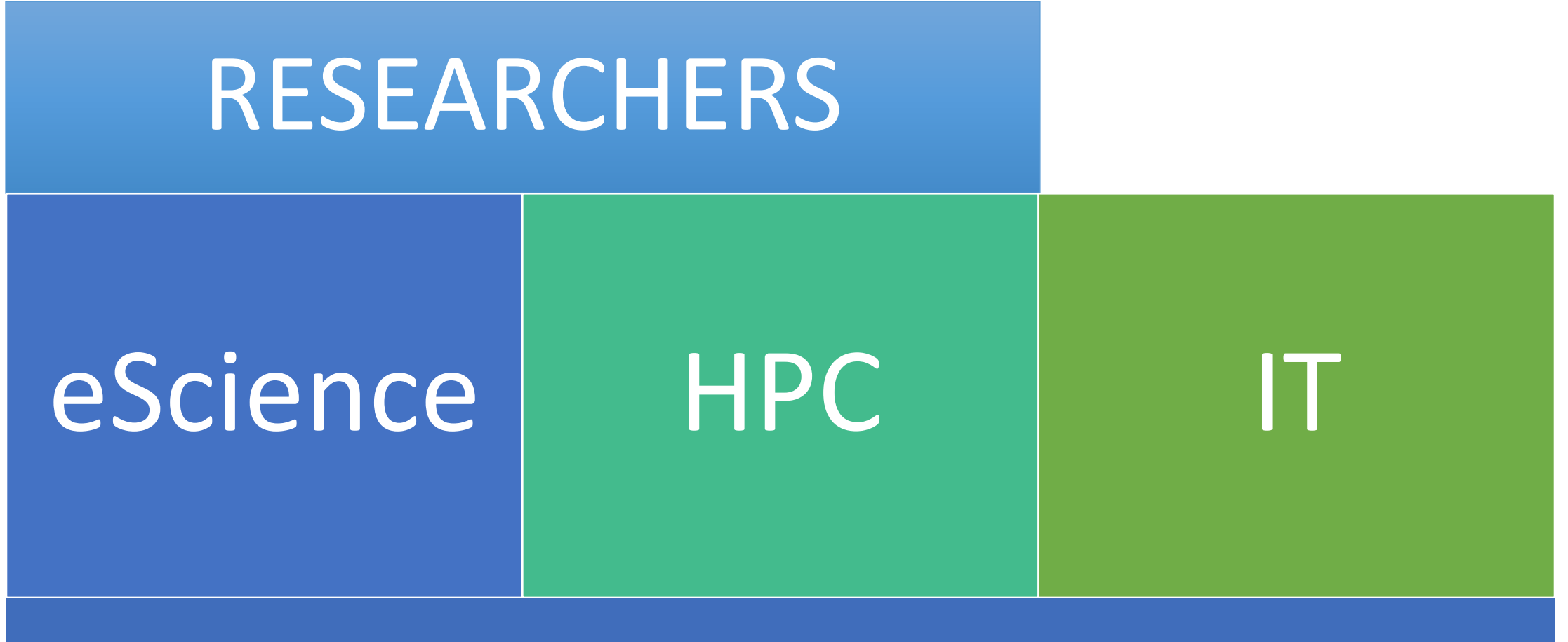
eScience+HPC+IT

RESEARCHERS

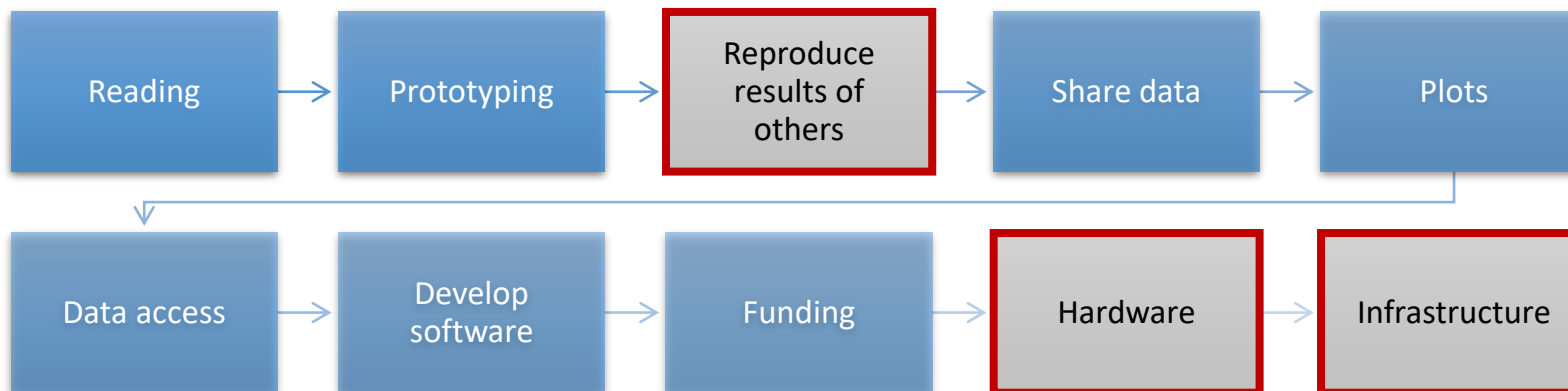
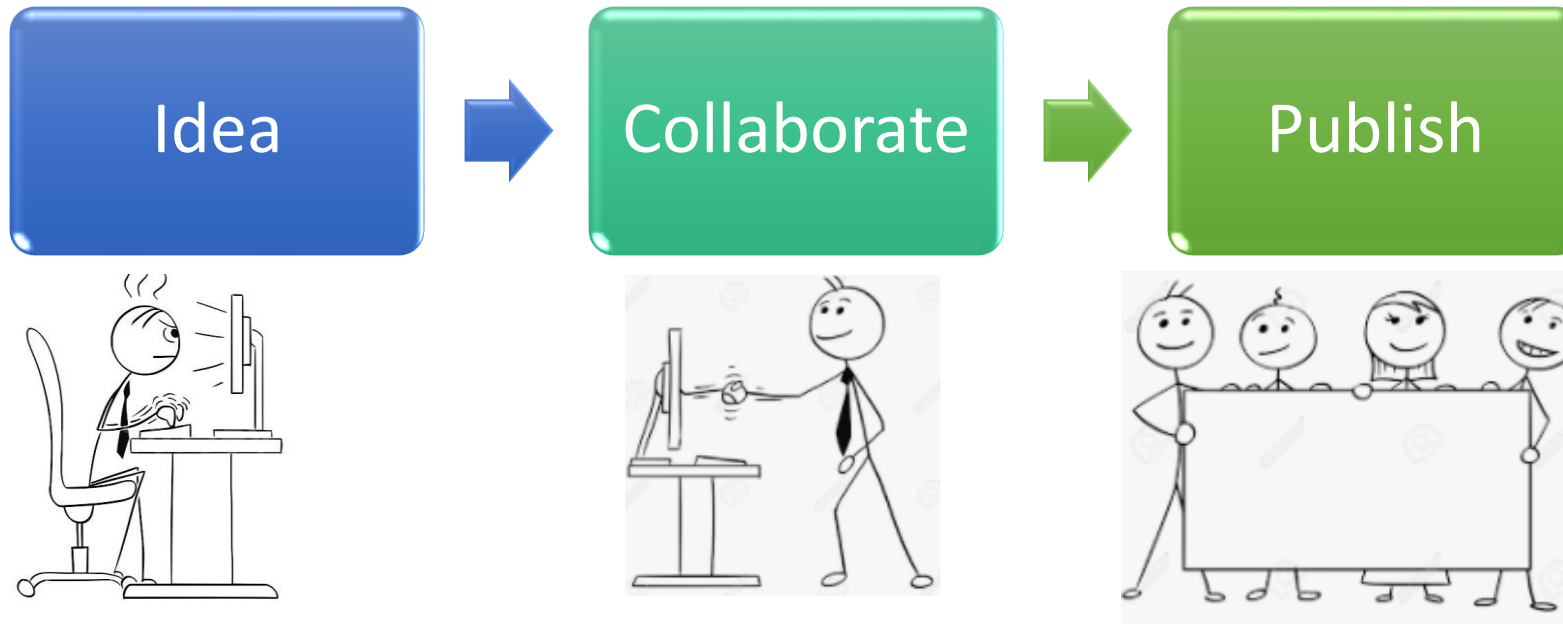
eScience

HPC

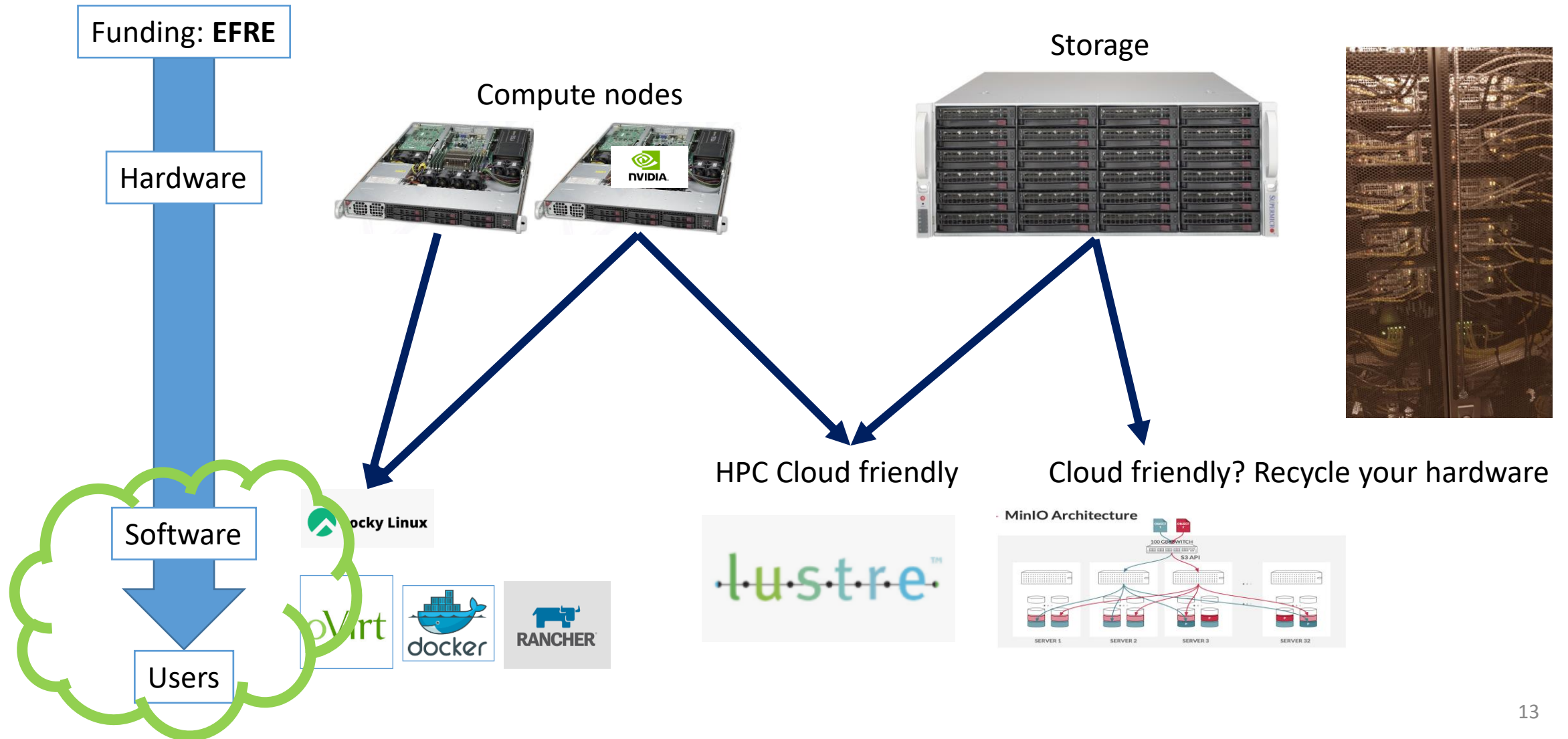
IT



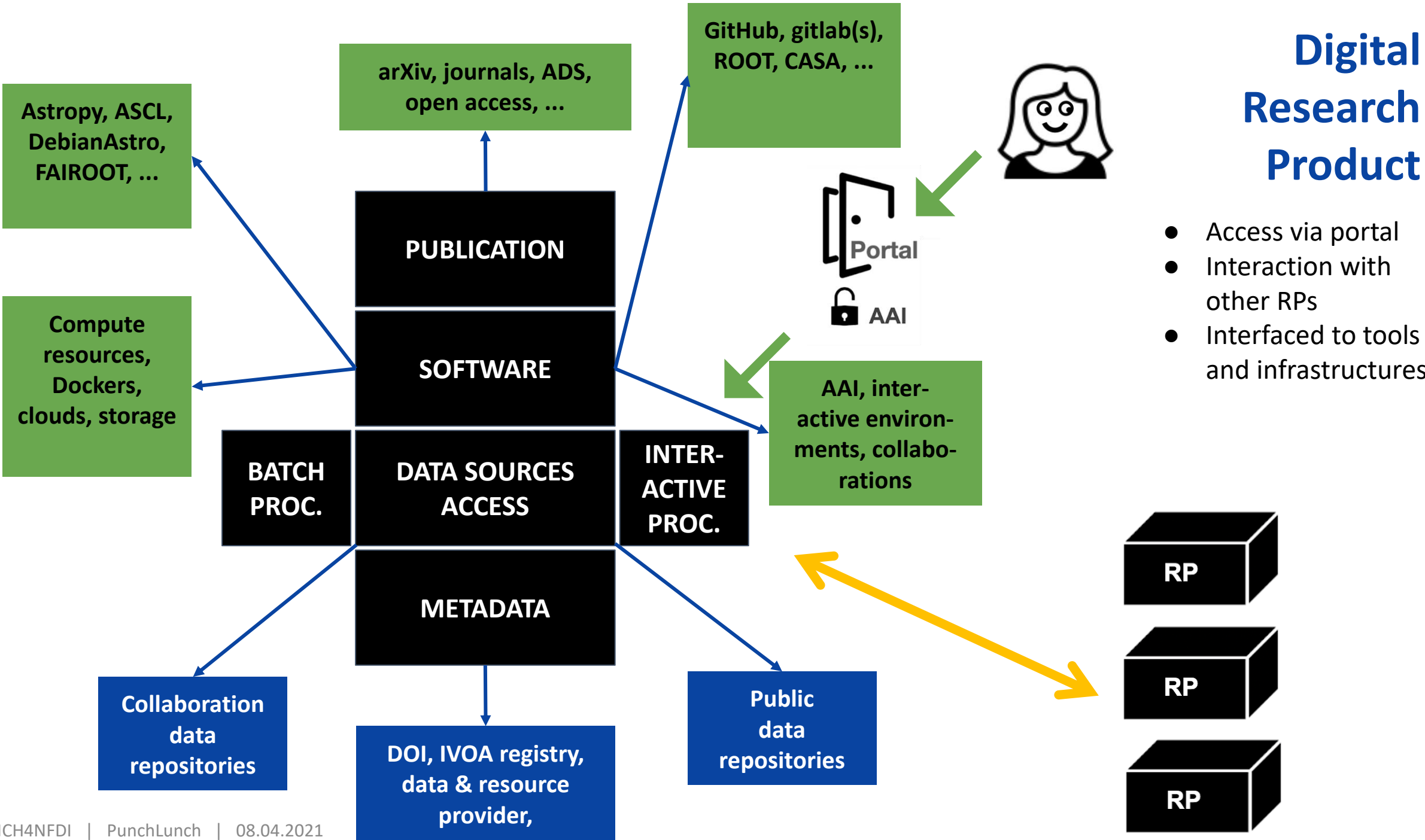
Scientific life (top to down)



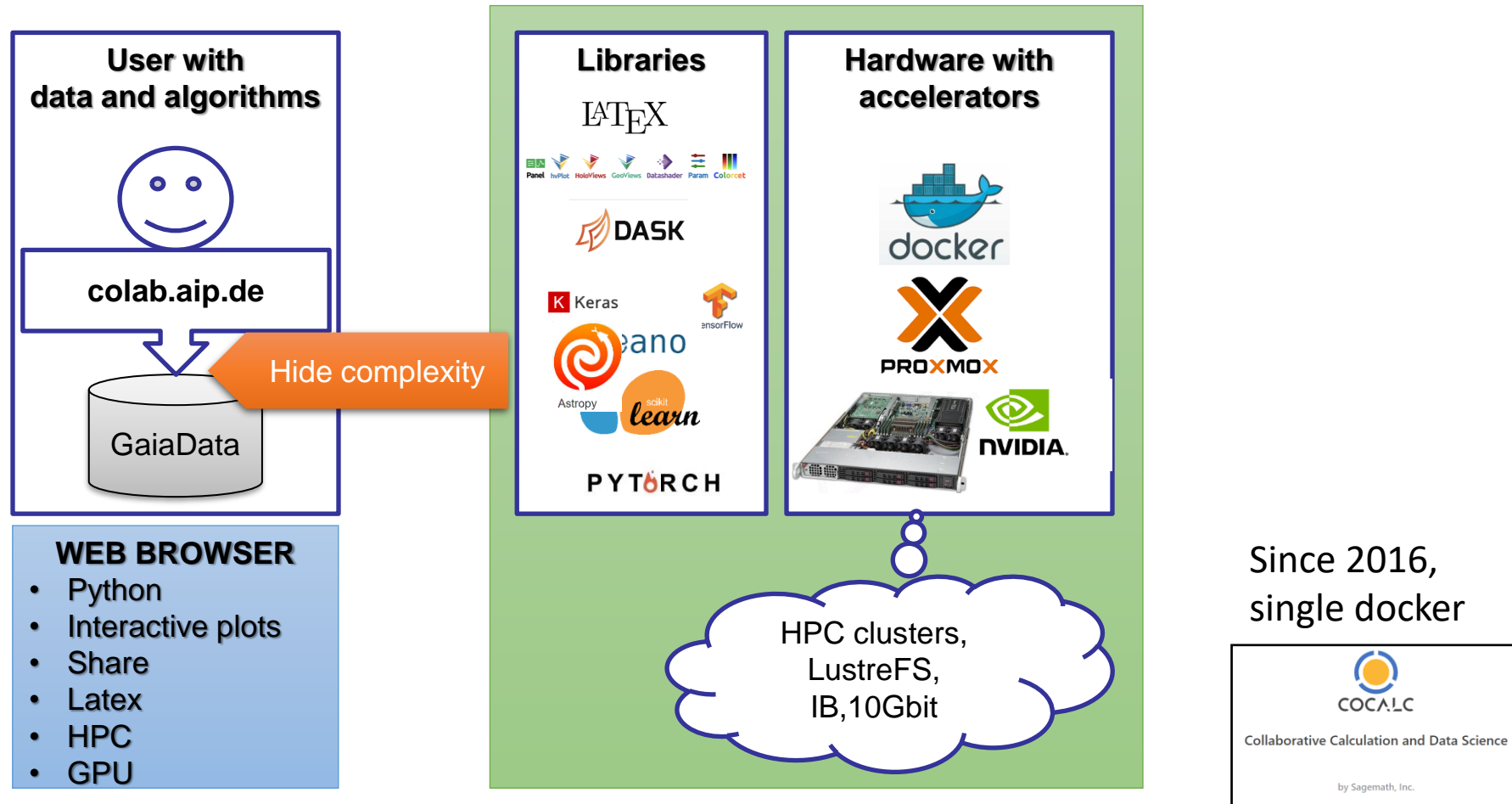
Infrastructure (down to top)



Digital Research Product



What we did at AIP before 2023?



CoCalc Integrated Tool: LLM as an assistant

The screenshot displays the CoCalc interface. On the left, a Jupyter Notebook titled '2023-04-25-file-1.ipynb' is open. The code in the notebook is as follows:

```
In [4]: import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

# Set the parameters
a = 2
b = 4

# Generate x-values
x = np.linspace(2015, 2020, 100)

# Calculate the y-values
y = a * x + b

# Create the plot
plt.figure(figsize=(8, 6))
plt.plot(x, y, color='red', linewidth=2)

plt.xlabel('Year')
plt.ylabel('Sales')
plt.title('Sales Data with Linear Trend')
plt.grid()
plt.show()
```

The output of the code is a line plot titled 'Sales Data with Linear Trend'. The x-axis is labeled 'Year' and the y-axis is labeled 'Sales'. The plot shows a red line representing a linear trend. The y-axis has major ticks at 4042 and 4044.

On the right side of the interface, a chat window is open. The chat history shows a message from '@Claude 3 Haiku 8k' asking for an example of a Python plot with a red linear line $f(x) = ax + b$ where a and b are free parameters like 2 and 4. The chat window also shows the code from the notebook and the resulting plot.

- ai.aip.de hosting local LLM at AIP
- Based on ollama
- And more...

- colab.aip.de: 250 users, over 900+ projects over 6 years
- Ai.aip.de: over 75 users in 3 weeks

The whole complexity is obscured from the users

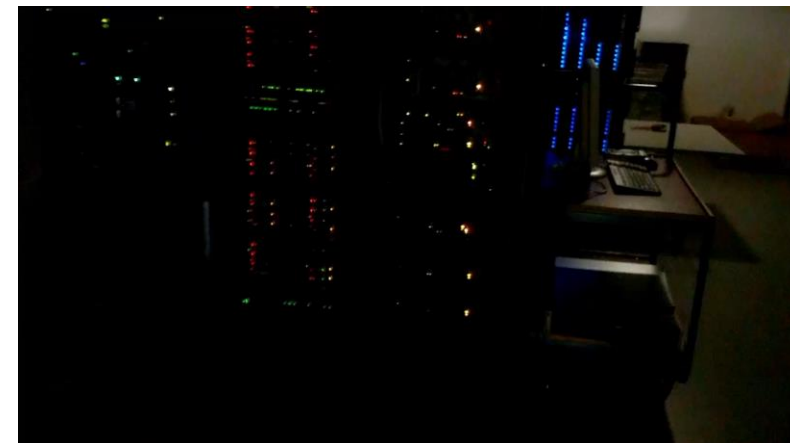
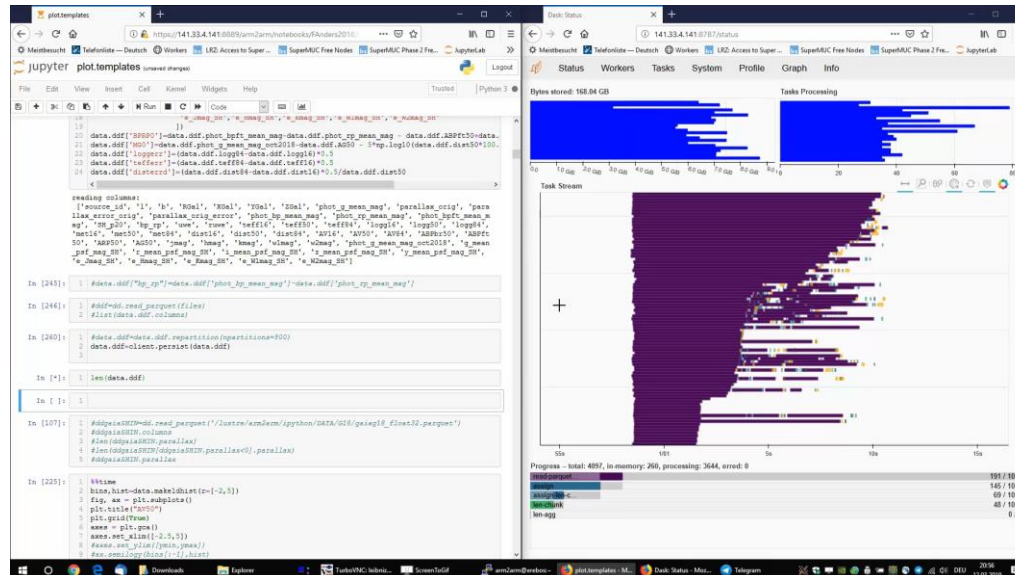
Users want the all tools in one place

- Data+LaTeX+Code
- Collaborators to share
- Article versions
- Cluster access
- Easy publishing for the demo notebooks

Possible solution:

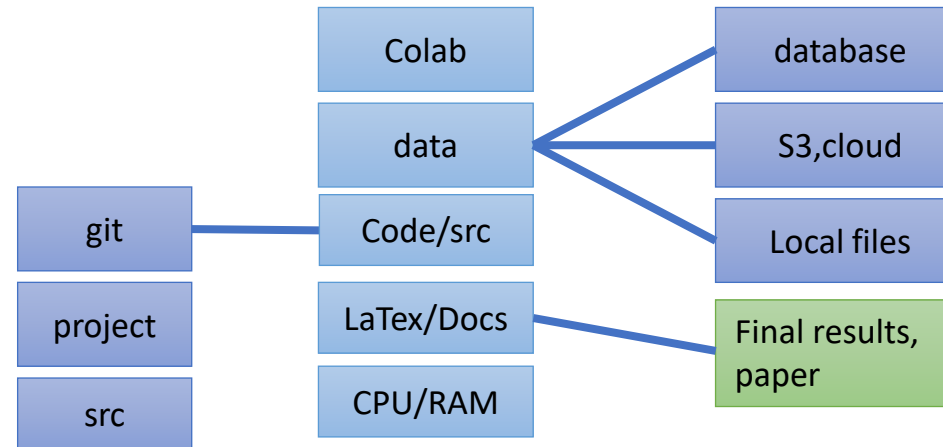
- dask+Kubernetes
- CoCalc project

CoCalc is a web-based cloud computing and course management platform for computational mathematics. Part of the Sage project, it supports editing of Sage worksheets, LaTeX documents and Jupyter notebooks.



Global Workflow of StarHorse team

A Bayesian code to estimate the photo-astrometric distances, extinctions, and astrophysical parameters for Gaia DR2 stars
F.Anders et al. (2019)



Getting the data

Get the list of the files: `wget --no-check-certificate http://data.aip.de/data/starhorse/fits/list-fits.txt`

Download the data: `wget --no-check-certificate -i list-fits.txt`

- Access examples: [starhorse_db](#)
- `cmd_from_db`: [launch binder](#) [Launch on Google Colab](#)
- `cmd_from_db_chunking`: [launch binder](#) [Launch on Google Colab](#)

<https://data.aip.de/projects/starhorse2019.html>

6 weeks 3000 cores get
400 000 000 Stellar parameters

What we learn from notebooks+jupyter?

- No versioning (even py codes are not versioned)
- No git (it is somehow possible but no one does this)
- No share
- No modularity
- 2-3 years cant run, for got the parameters in the cell.
- Astronomers during prototyping are writing terrible codes.

What about kubernetes?

- in Astrophysics infrastructure we are still in the same stage as “**Docker Inc.**” was in **2014**.

Why?

- It was complex
- Rapid development in the Industry
- No LTS

Situation is matured in 2021:

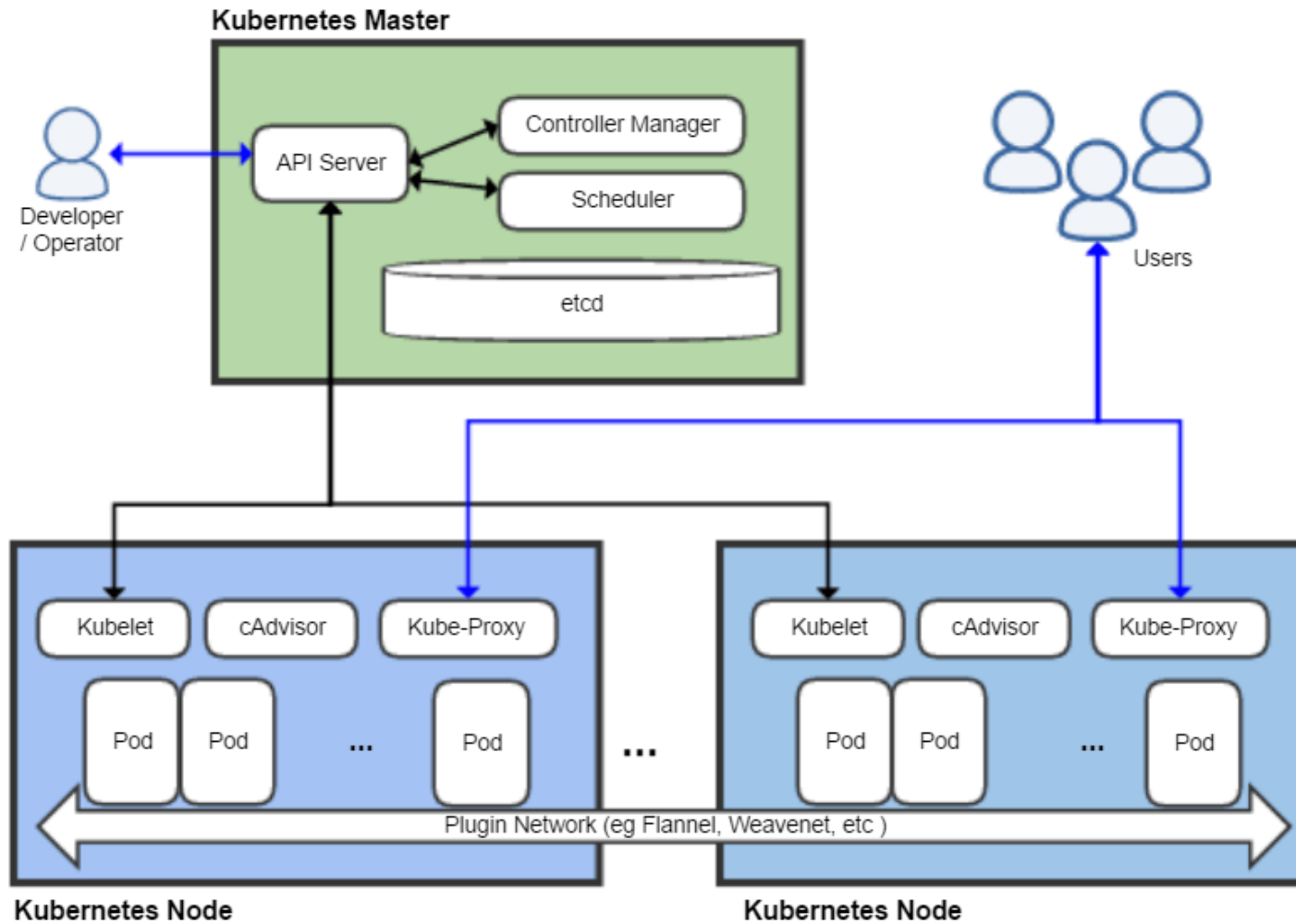
- Because of <https://www.cncf.io/>



- We are ready to adopt some Infa from industry into to scientific life



Kubernetes



Are we special?
Users images are so huge they are filling local host disks

Microservices: Reproducible science

Use Cases at AIP

- **Colab.aip.de**
 - Quotas
 - Project isolation
- **Data analysis pipelines with versioning**
 - Reproducible science
 - Pipeline versioning
 - GaiaDR1,2,3
 - RAVEDR1-6
 - StarHorse-18,19,20
- **Publish papers with interactive plots**
 - like binder
 - Example: distill.pub by google
- **Dynamically Scalable webpages**
- **gitlabs @ aip**: CI integration

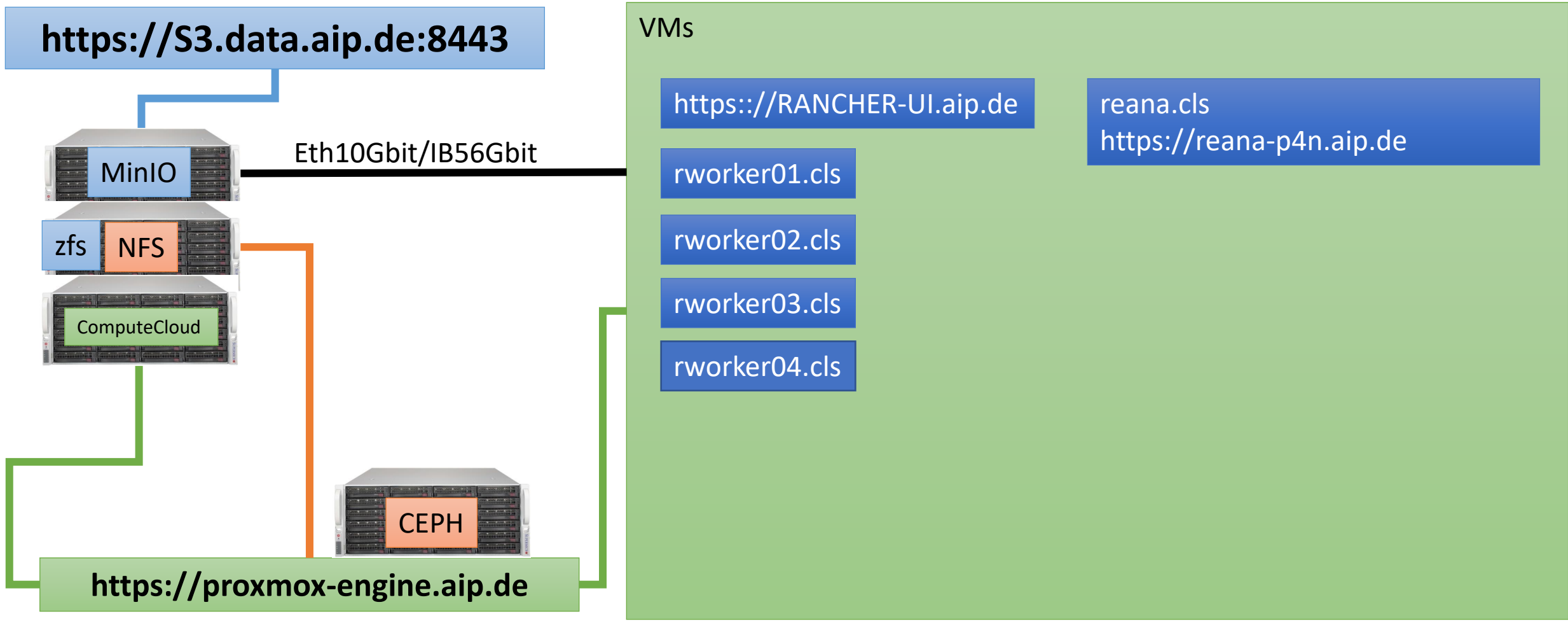
Pros:

- *Direct GIT integration*
- *Scalability*
- Modularity
- Distributed development
- Integration
- Save resources/power

Concerns:

- Complexity
- Design
- *Testing, debugging*
- *Inter-service call latency*

REANA: Infra



RANCHER Only User Namespaces

Home

EXPLORE CLUSTER

Type to search clusters

- aipkub
- ckube24
- colab24
- local

GLOBAL APPS

- Continuous Delivery
- Cluster Management
- Virtualization Management

CONFIGURATION

- Users & Authentication
- Extensions
- Global Settings

Installed App: reanadev Deployed

Namespace: reanadev Age: 216 days

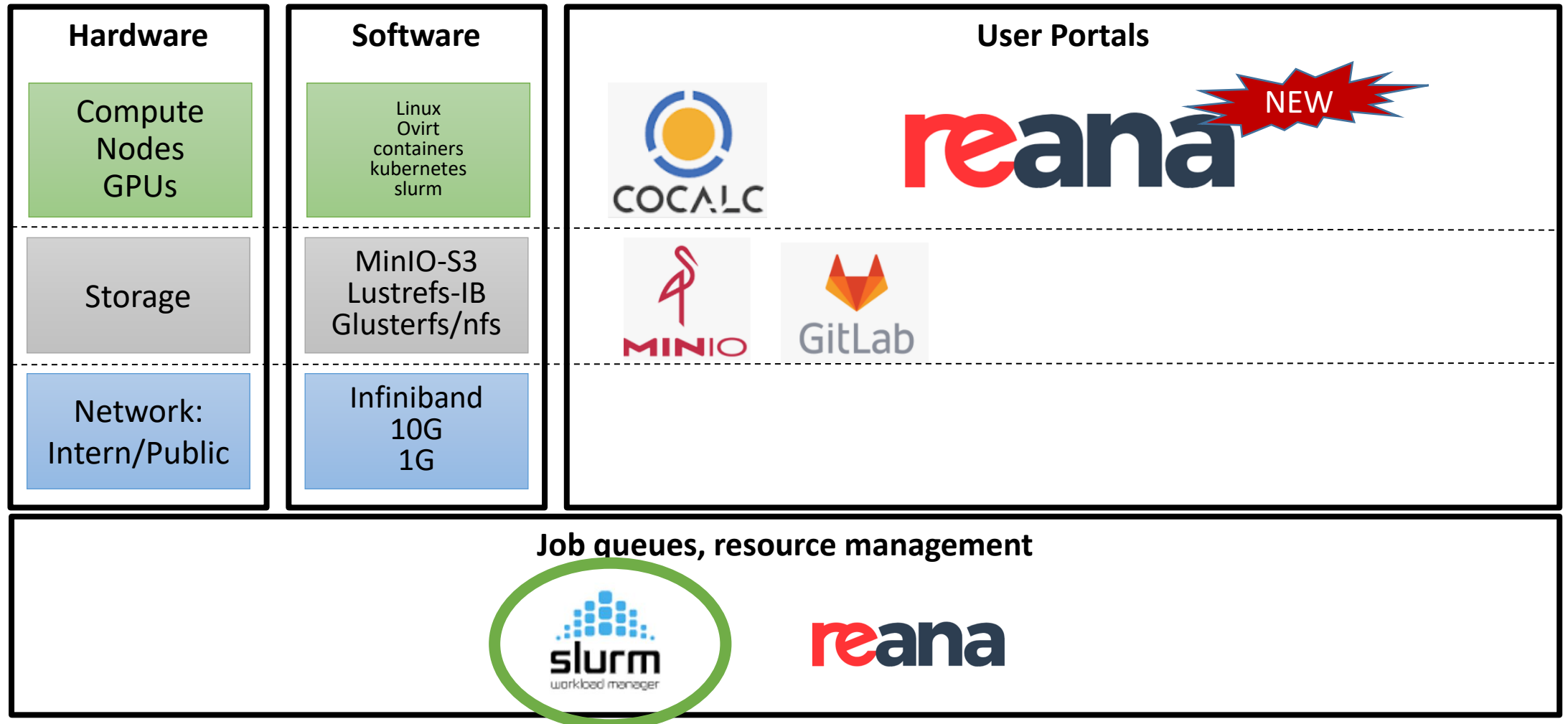
Deployed: 57 days

sources Values YAML Chart README Release Notes

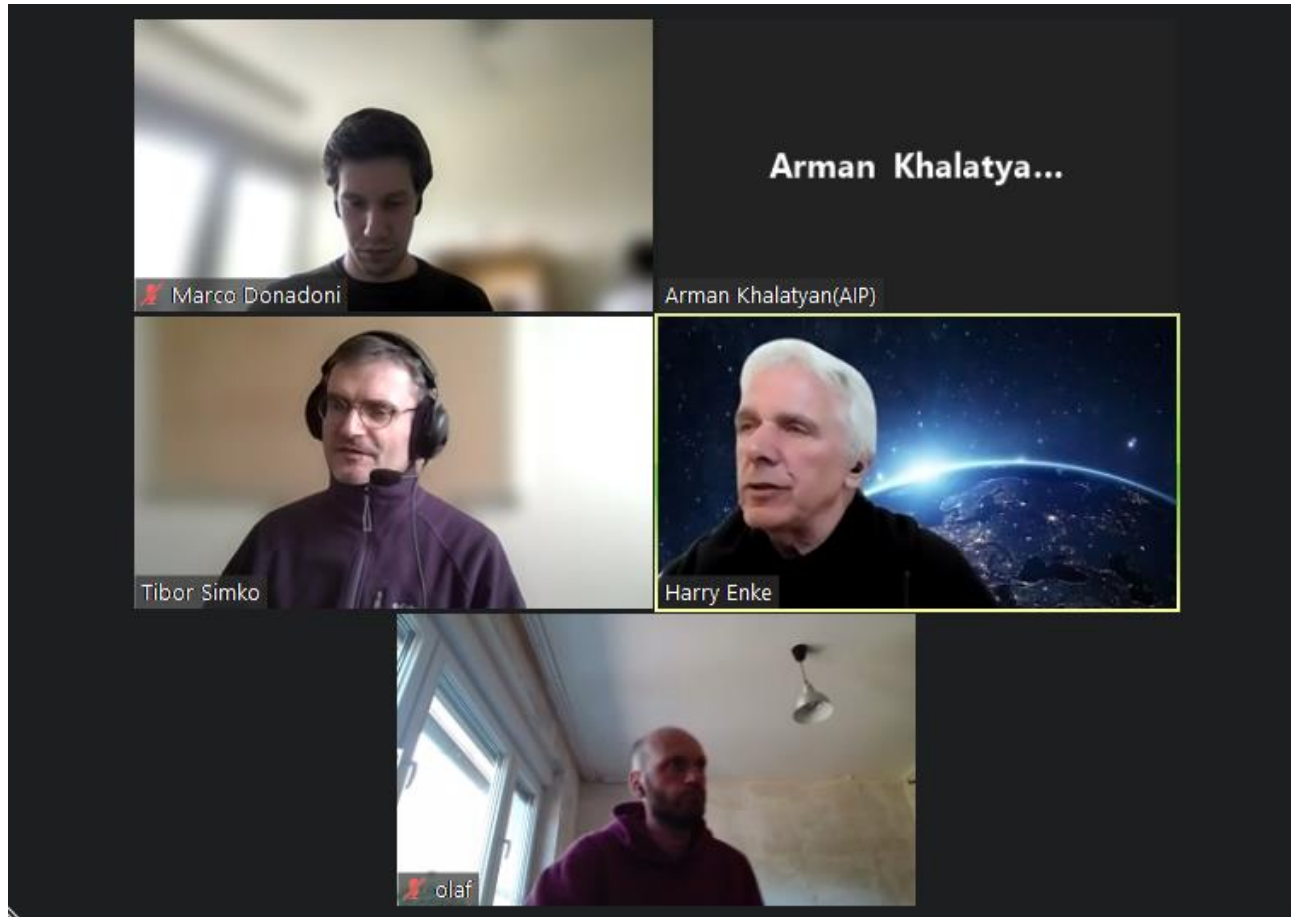
State	Type	Name	Namespace
Active	ConfigMap	reana-config	reanadev
Active	Service	reanadev-cache	reanadev
Active	Deployment	reanadev-cache	reanadev
Active	Secret	reanadev-cern-gitlab-secrets	reanadev
Active	Secret	reanadev-cern-sso-secrets	reanadev
Active	Service	reanadev-db	reanadev
Active	Deployment	reanadev-db	reanadev

```
helm install reanadev24 reanahub/reana --create-namespace -n reanadev24 -f values.yaml
```

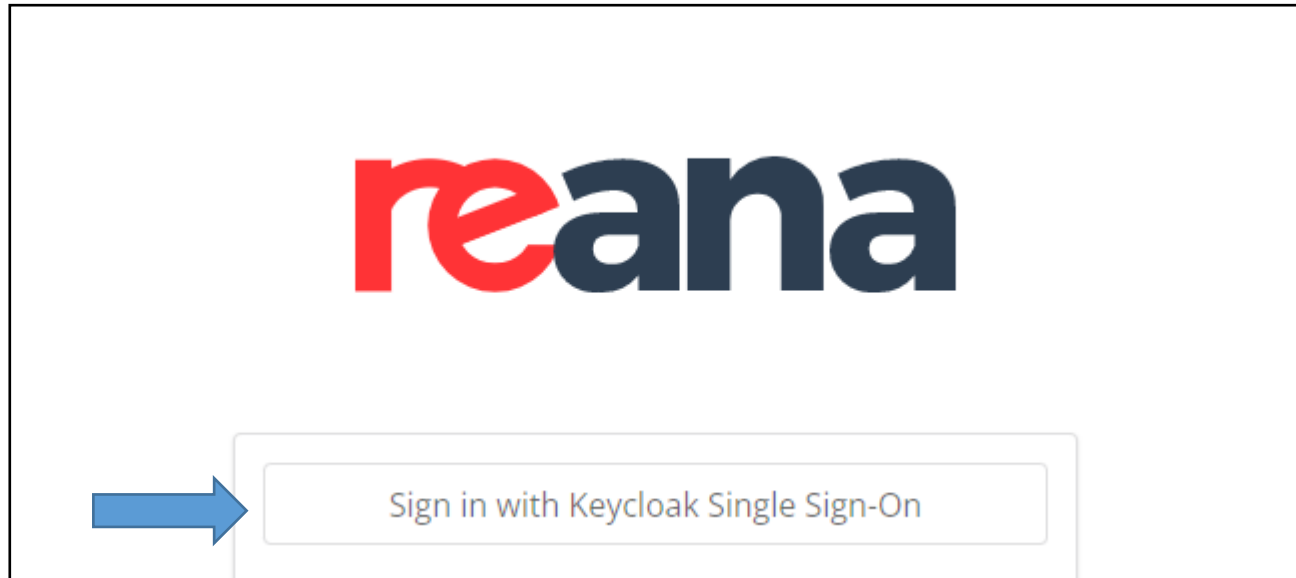
SAAS, IAAS and PAAS



REANA and AIP discussion rounds



REANA: in Action

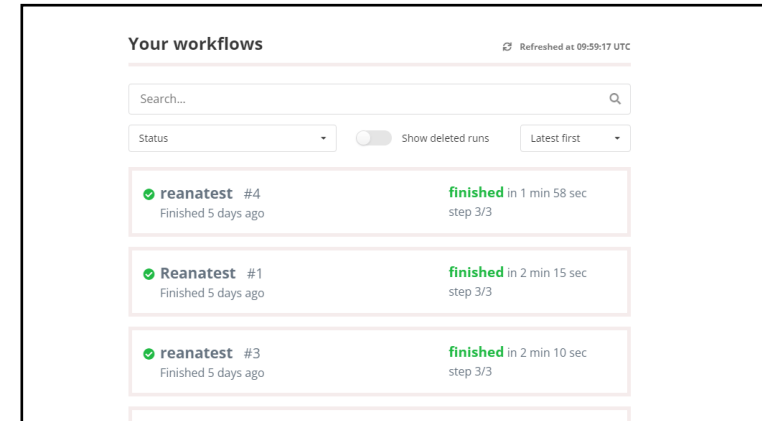


<https://reana-p4n.aip.de/>

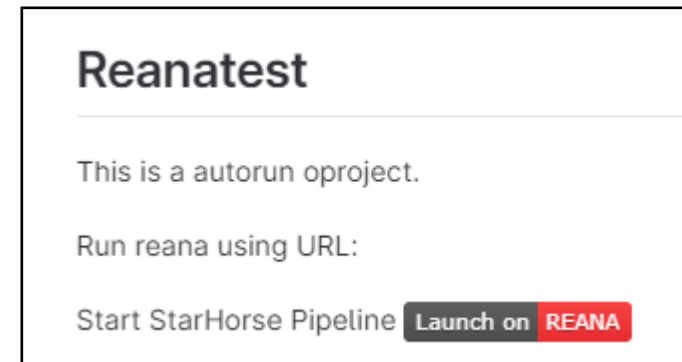
Use **reana-client** from terminal

Connect to gitlab

<https://gitlab-p4n.aip.de/arm2arm/reanatest>



Launch from URL



REANA hosting arbitrary webpage

reana-p4n.aip.de/ee373510-c71c-4660-91f1-d0e9a9a33dbd/?token=WW-Z7HoRm3q_3sdBVIBNyQ

REANA@AIP examples Gallery

search

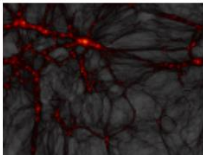
Render python(Not ready)

Render OpenGL(Not ready)

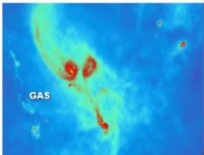
Low metallicity stars(Not ready)

Mollweide FoV for widefield plates

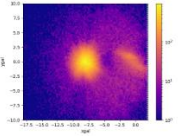
Render python(Not ready)
Render cosmological simulation



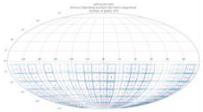
Render OpenGL(Not ready)
PMViewer interactive rendering of the cosmological simulation



Low metallicity stars(Not ready)
GAIA-DR3 data access to find the low metallicity stars inside the StarHorse database.



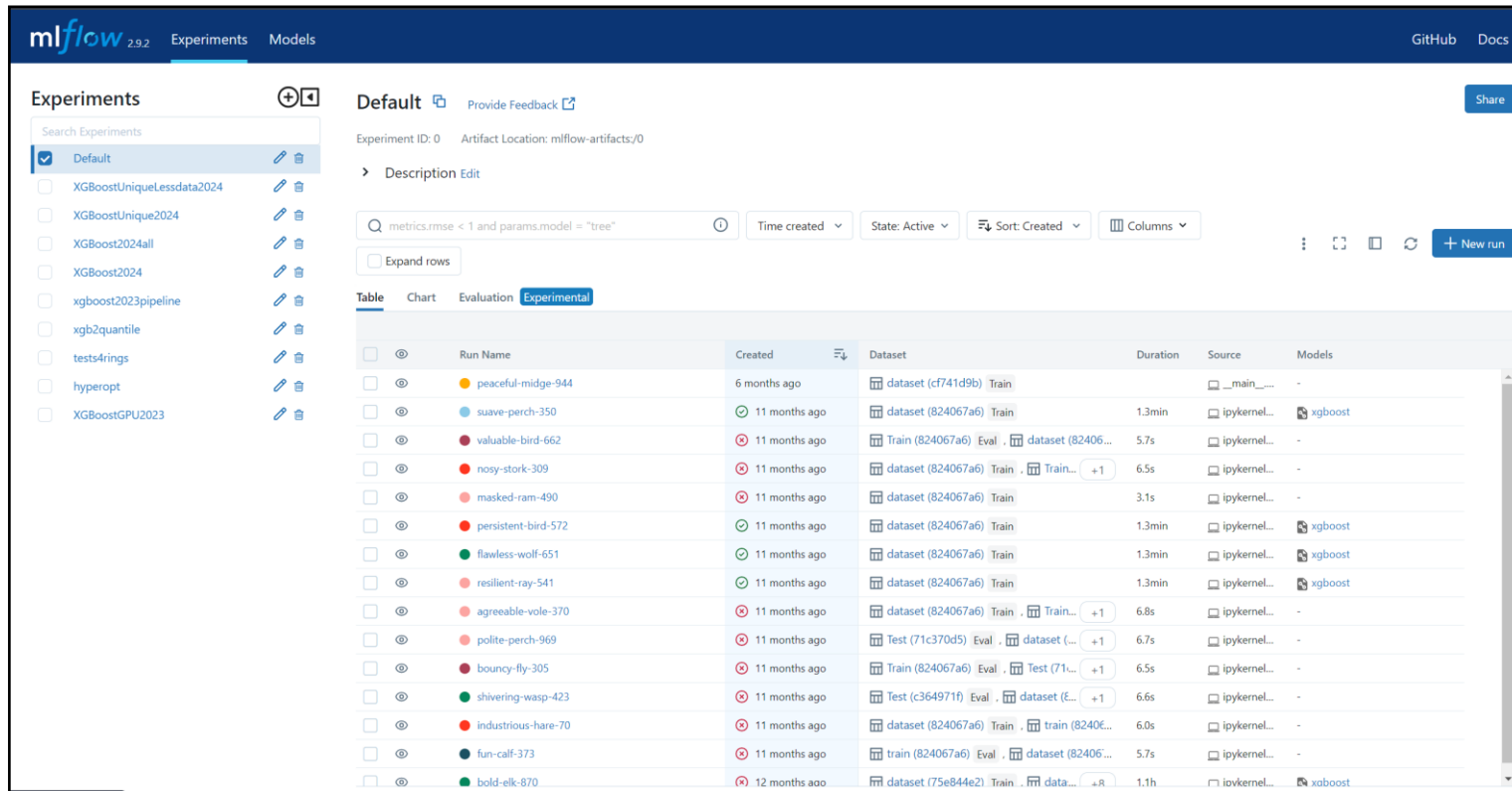
Mollweide FoV for widefield plates
Extract with TAP from astronomical database and plot the FoV / coverage for the archives.



Custom images are available on NFDI4PUNCH git:
<https://gitlab-p4n.aip.de/>

reana-jailbreak?

MLFlow: as a ML experiments server



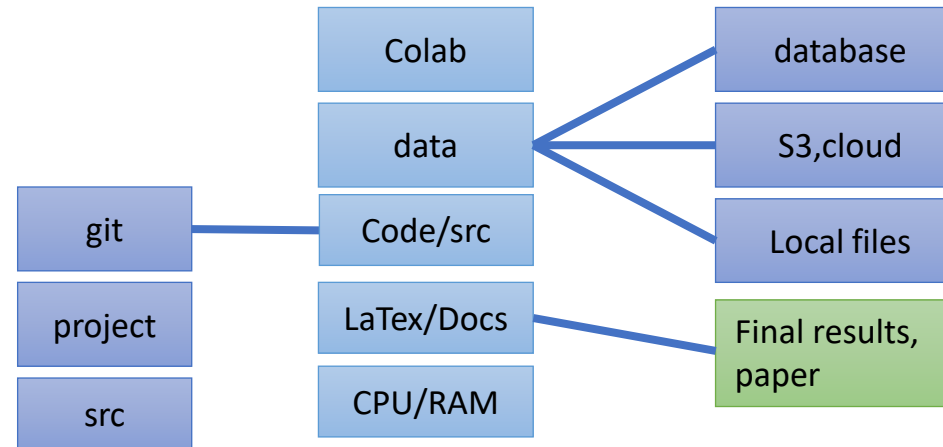
The screenshot displays the MLFlow Experiments page. On the left, there is a sidebar with a search bar and a list of experiments, including 'Default' (selected), 'XGBoostUniqueLessdata2024', 'XGBoostUnique2024', 'XGBoost2024all', 'XGBoost2024', 'xgboost2023pipeline', 'xgb2quantile', 'tests4rings', 'hyperopt', and 'XGBoostGPU2023'. The main area shows the 'Default' experiment details, including the experiment ID (0) and artifact location (mlflow-artifacts/0). Below this, there is a search bar with the query 'metrics.rmse < 1 and params.model = "tree"', a 'Time created' dropdown, a 'State: Active' dropdown, a 'Sort: Created' dropdown, and a 'Columns' dropdown. A 'New run' button is visible. The main content is a table of runs with the following columns: Run Name, Created, Dataset, Duration, Source, and Models. The table contains 20 rows of runs, each with a unique name and various attributes.

Run Name	Created	Dataset	Duration	Source	Models
peaceful-midge-944	6 months ago	dataset (cf741d9b) Train		__main_...	-
suave-perch-350	11 months ago	dataset (824067a6) Train	1.3min	ipykernel...	xgboost
valuable-bird-662	11 months ago	Train (824067a6) Eval, dataset (82406...	5.7s	ipykernel...	-
nosy-stork-309	11 months ago	dataset (824067a6) Train, Train... +1	6.5s	ipykernel...	-
masked-ram-490	11 months ago	dataset (824067a6) Train	3.1s	ipykernel...	-
persistent-bird-572	11 months ago	dataset (824067a6) Train	1.3min	ipykernel...	xgboost
flawless-wolf-651	11 months ago	dataset (824067a6) Train	1.3min	ipykernel...	xgboost
resilient-ray-541	11 months ago	dataset (824067a6) Train	1.3min	ipykernel...	xgboost
agreeable-vole-370	11 months ago	dataset (824067a6) Train, Train... +1	6.8s	ipykernel...	-
polite-perch-969	11 months ago	Test (71c370d5) Eval, dataset (... +1	6.7s	ipykernel...	-
bouncy-fly-305	11 months ago	Train (824067a6) Eval, Test (71... +1	6.5s	ipykernel...	-
shivering-wasp-423	11 months ago	Test (c364971f) Eval, dataset (E... +1	6.6s	ipykernel...	-
industrious-hare-70	11 months ago	dataset (824067a6) Train, train (82406...	6.0s	ipykernel...	-
fun-calf-373	11 months ago	train (824067a6) Eval, dataset (82406...	5.7s	ipykernel...	-
bold-elk-870	12 months ago	dataset (75e844e2) Train, data... +R	1.1h	iovkernel...	xgboost

- Can we deploy this within the reana?
- Answer: yes
- Security concerns...
- I loved:
 - Streamlit
 - MLflow
 - Panel
 - React native page

Coming Soon: Global Workflow of StarHorse team

Transferring spectroscopic stellar labels to 220 million Gaia DR3 XP stars with XGBoost



Getting the data

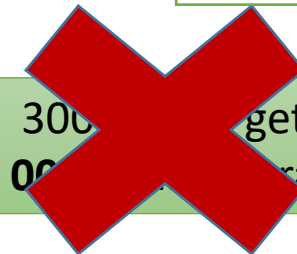
Get the list of the files: `wget --no-check-certificate http://data.aip.de/data/starhorse/fits/list-fits.txt`

Download the data: `wget --no-check-certificate -i list-fits.txt`

- Access examples: [starhorse_db](#)
- `cmd_from_db`: [launch binder](#) [Launch on Google Colab](#)
- `cmd_from_db_chunking`: [launch binder](#) [Launch on Google Colab](#)

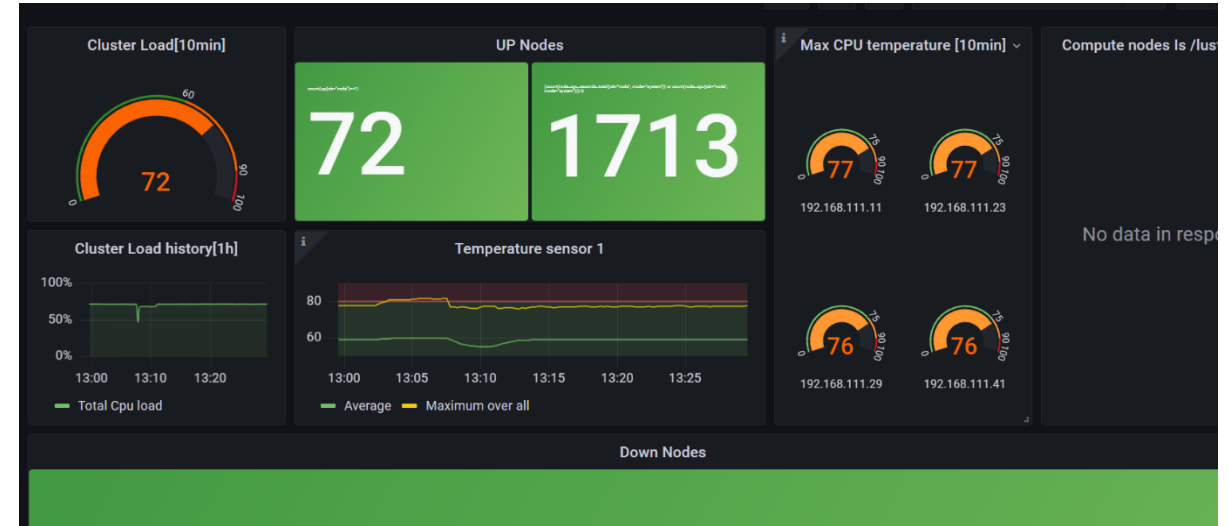
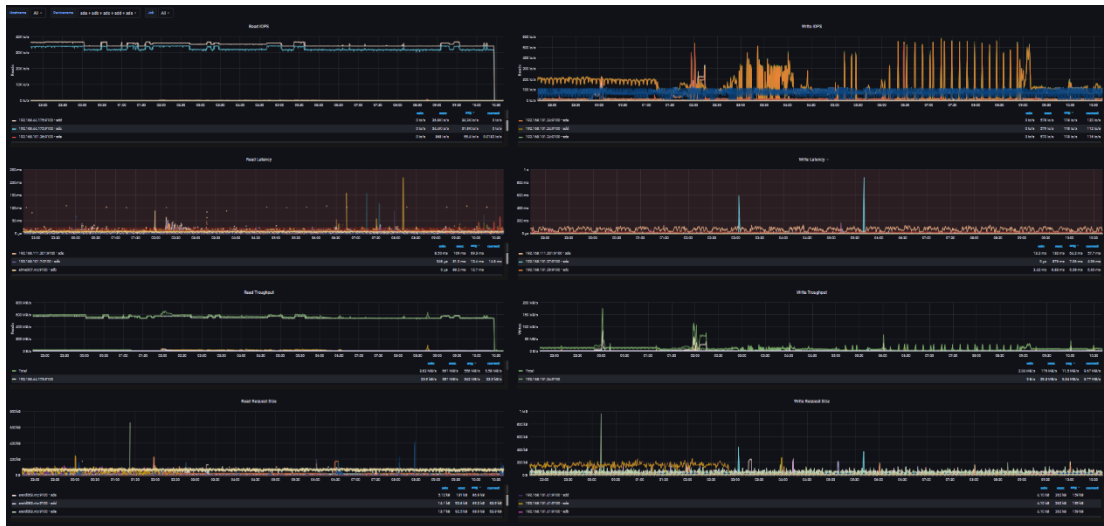
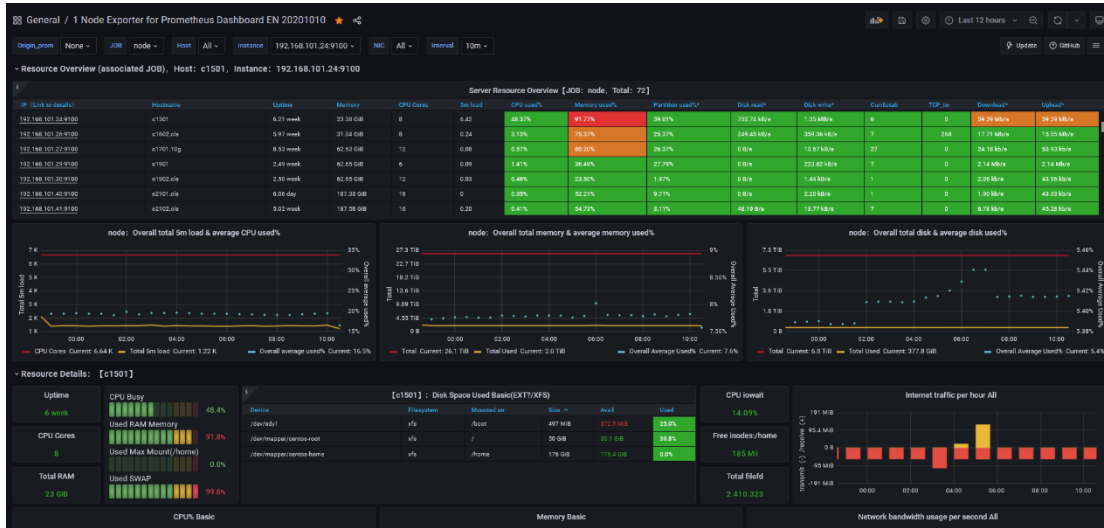
1 A100
1 week
Preparation 2 years

6 weeks 300 get
400 000 000 parameters



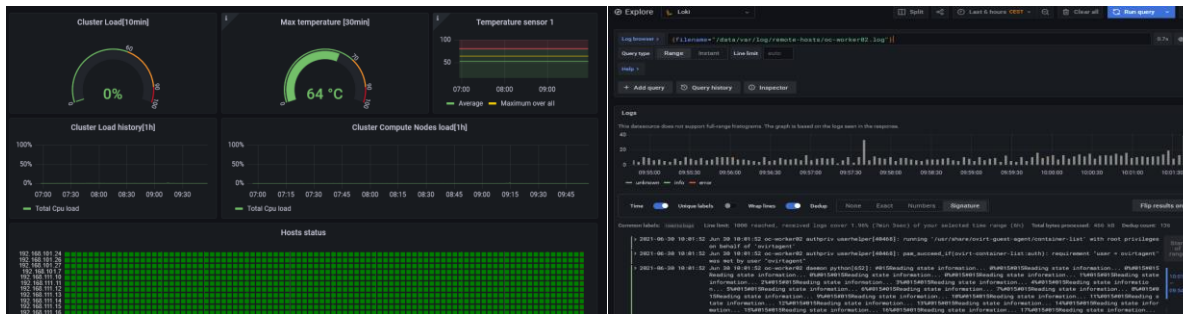
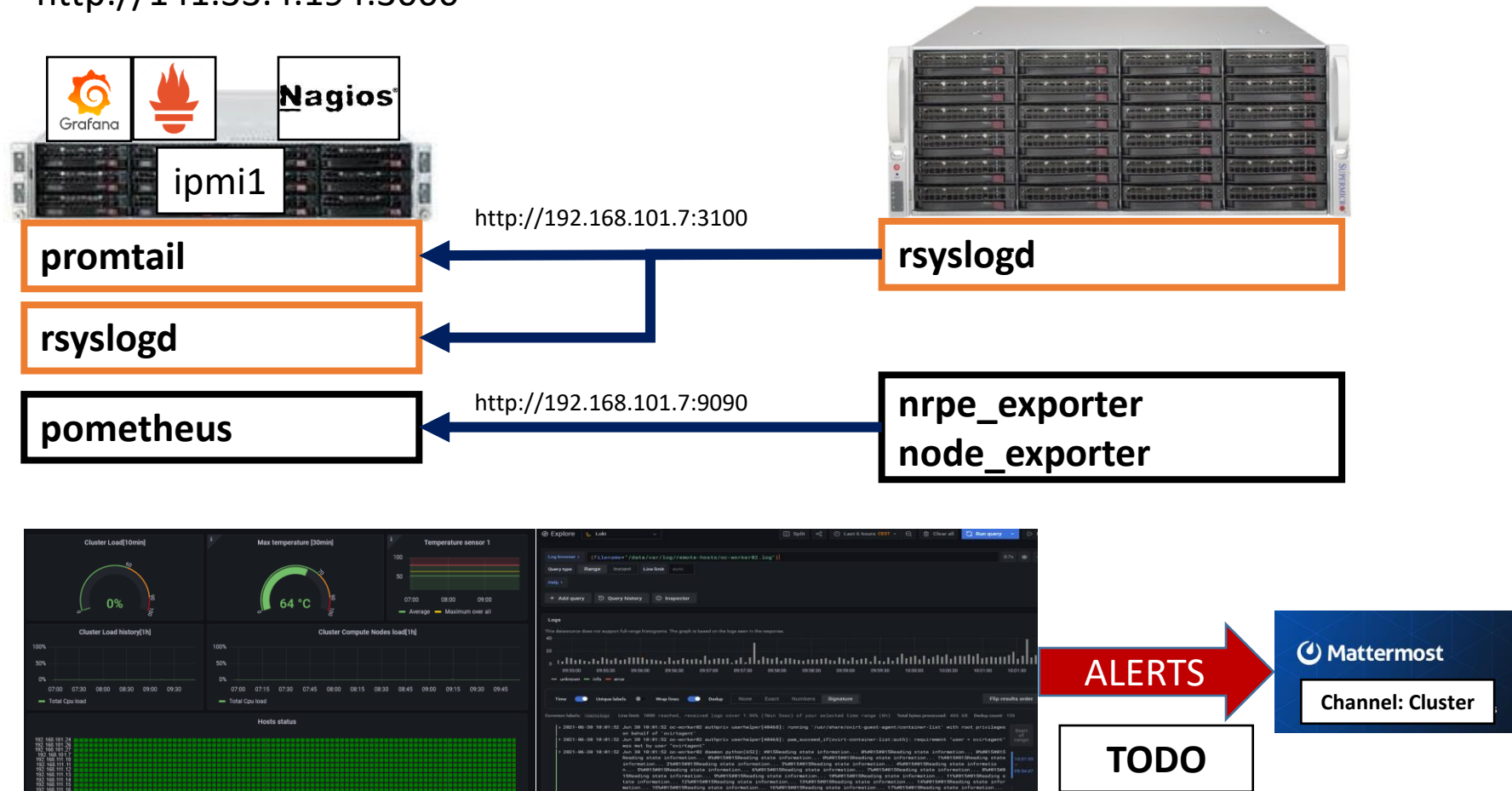
Monitoring is important!

Cluster Monitoring (Grafana)



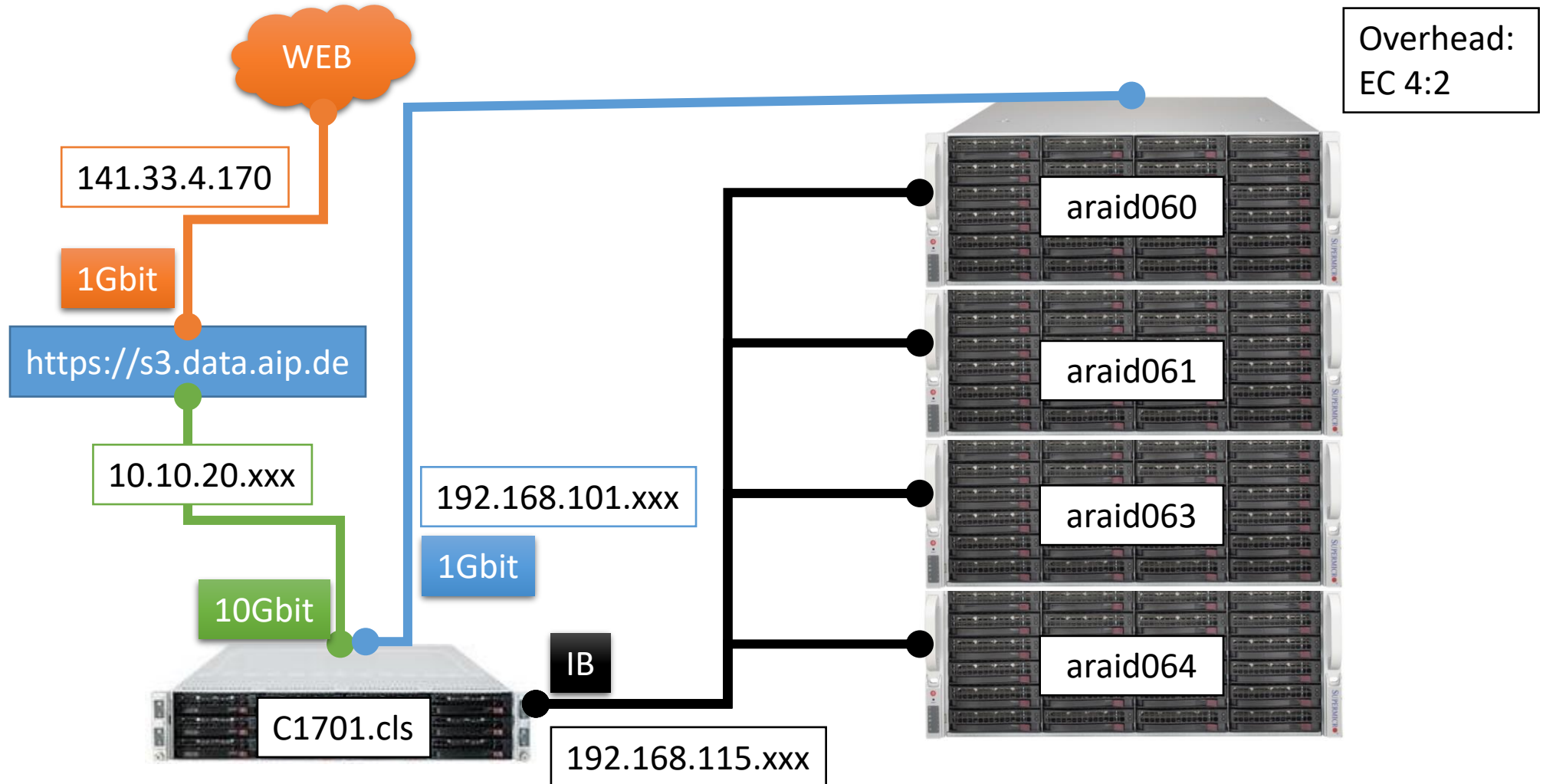
Monitoring stack

http://141.33.4.194:3000



Data management

S3 storage at AIP: MinIO network



Moving data from clusters?



REANA as a main ingredient for NFDI4PUNCH

- Helmholtz-AAI is integrated and working w/o problems
- Registered users: >50 users within 3 months
- We are looking for stability tests to announce at AIP
- Gitlab container registry as a main source for containers
- Dev steps:
 - Actively developing HT_Condor integration(Manuel)
 - Any SLURM backend(Arman,Elena)
 - Merging to REANA basecode(Tibor,Marco and team...)
- What is still missing:
 - Workflow shares
 - Data to(from) Storage workflows
 - Easy token management
 - Not implemented the LustreFS integration

~~Use CLOUD everywhere!!!~~



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Elena will demonstrate
how to use REANA with
S3 storage and more

Questions?