



PP&B – Computer Support Group

FRITZ-HABER-INSTITUT  
MAX-PLANCK-GESELLSCHAFT



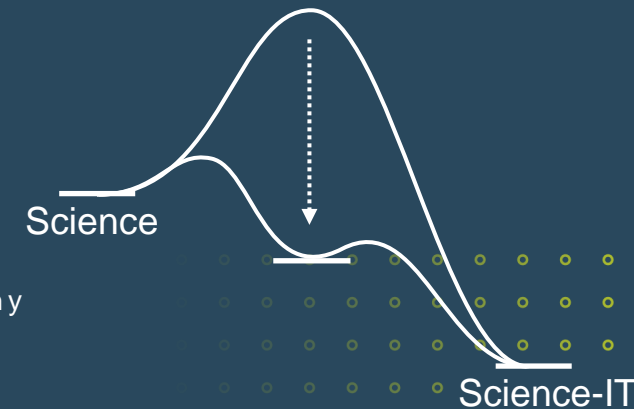
# THE FUTURE ROLE OF PP&B AT THE FHI

## TACKLING CURRENT AND FUTURE CHALLENGES OF SCIENTIFIC IT

Simeon D. Beinlich<sup>1,\*</sup> and Heinz Junkes<sup>1</sup>

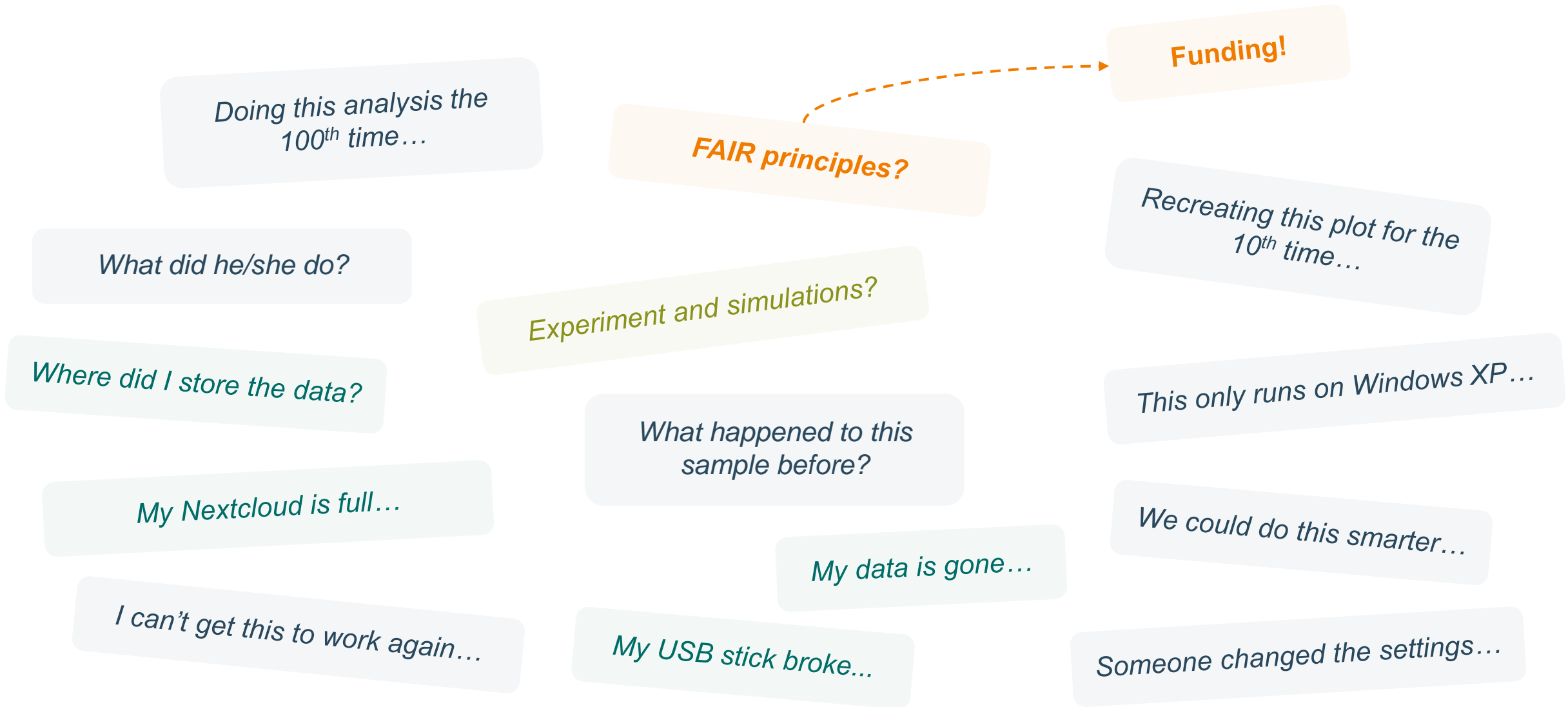
<sup>1</sup> PP&B – Computer Support Group  
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

\*beinlich@fhi.mpg.de





# (SOME) CHALLENGES IN SCIENTIFIC IT

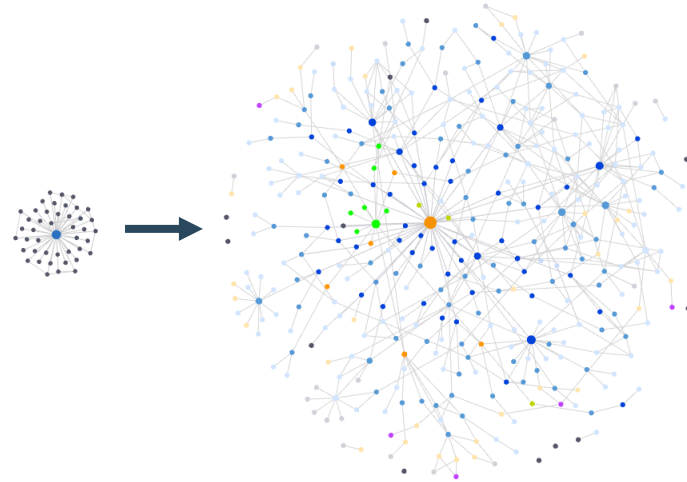




# CHALLENGES IN SCIENTIFIC IT

More data

More complex data



More complex analyses

More complex setups

More requirements



# CHALLENGES IN SCIENTIFIC IT

**More data**

**More complex data**

*... More IT ...*

**More complex analyses**

**More complex setups**

**More requirements**





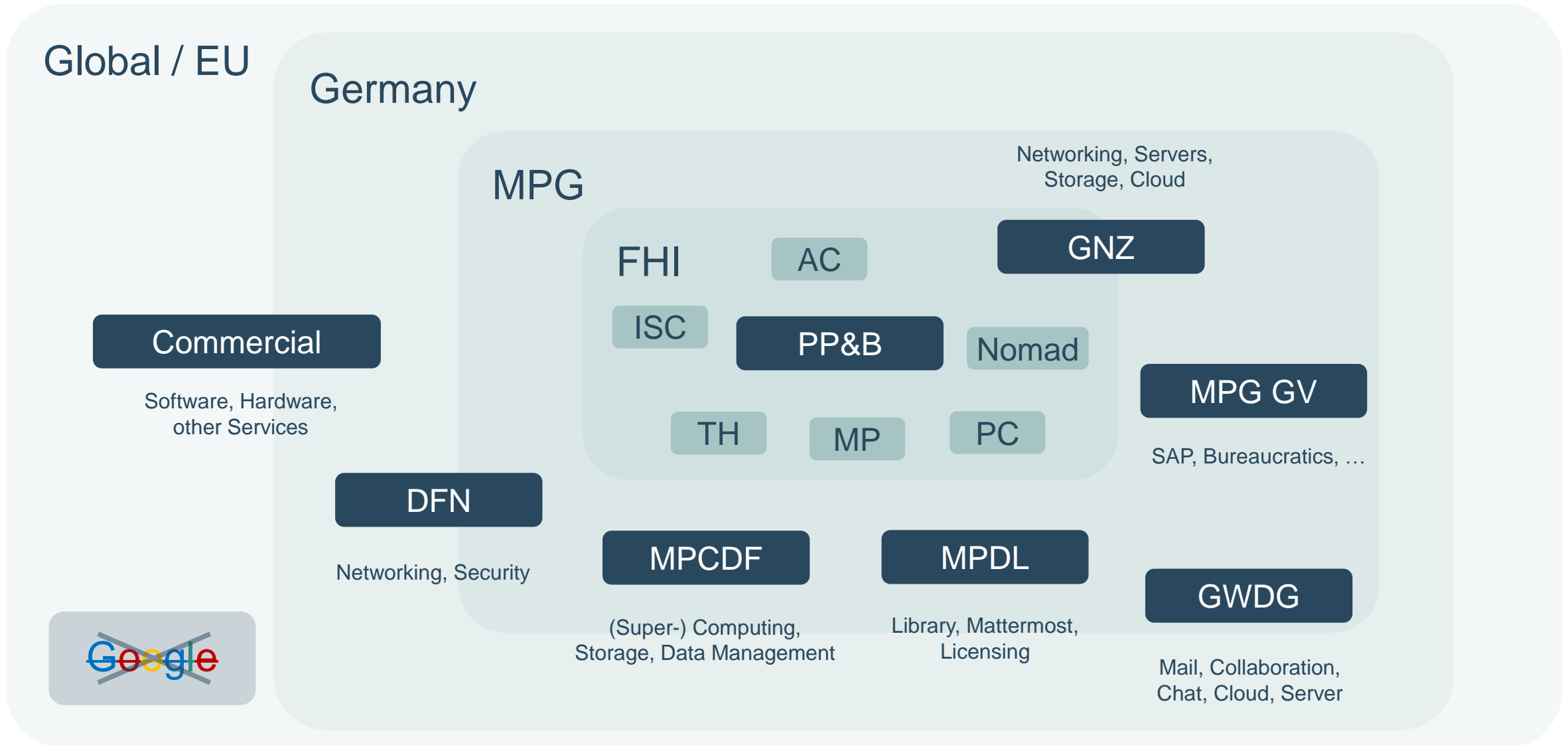
# IT INFRASTRUCTURE AT MPG & FHI

## &

# THE ROLE OF PP&B

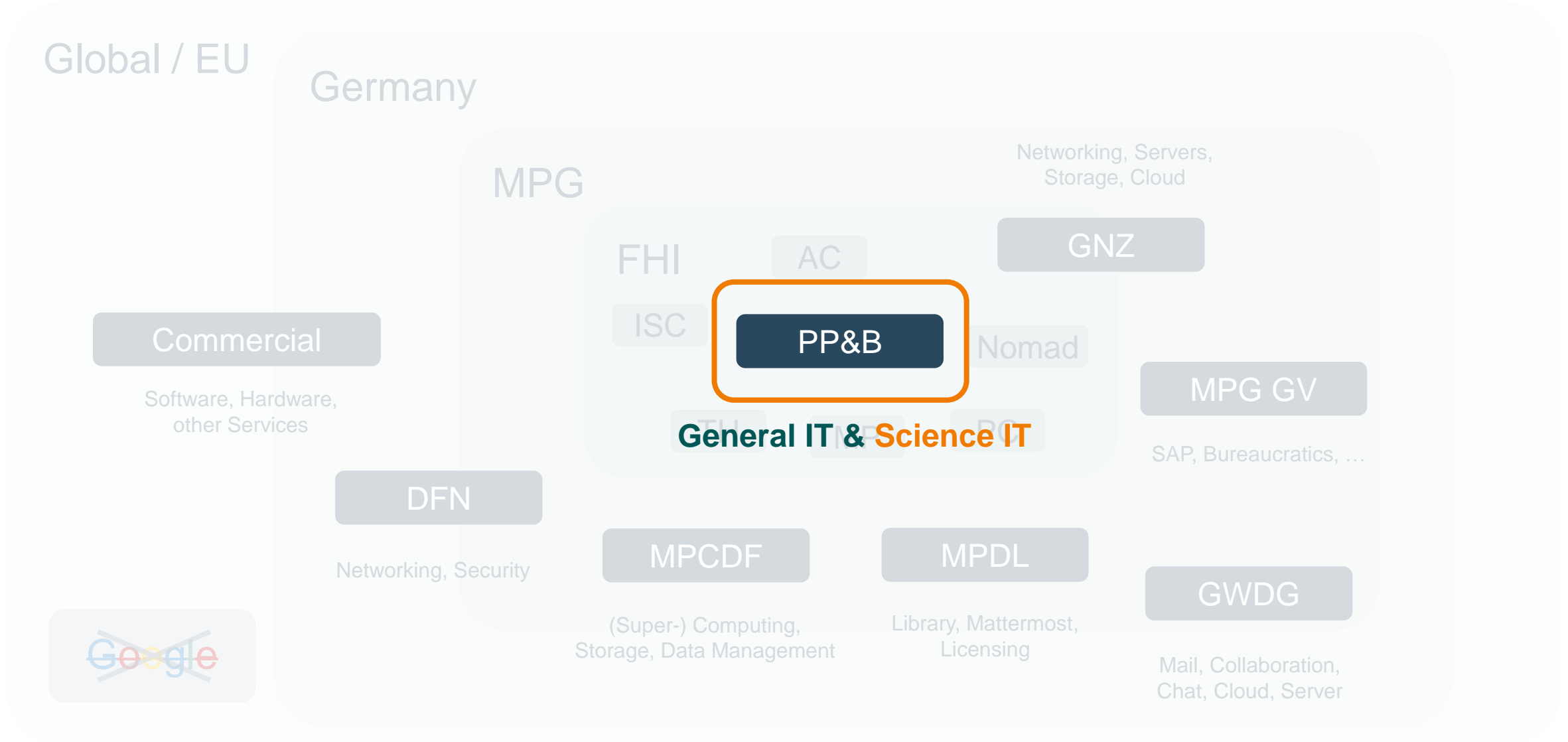


# IT INFRASTRUCTURE AT MPG & FHI



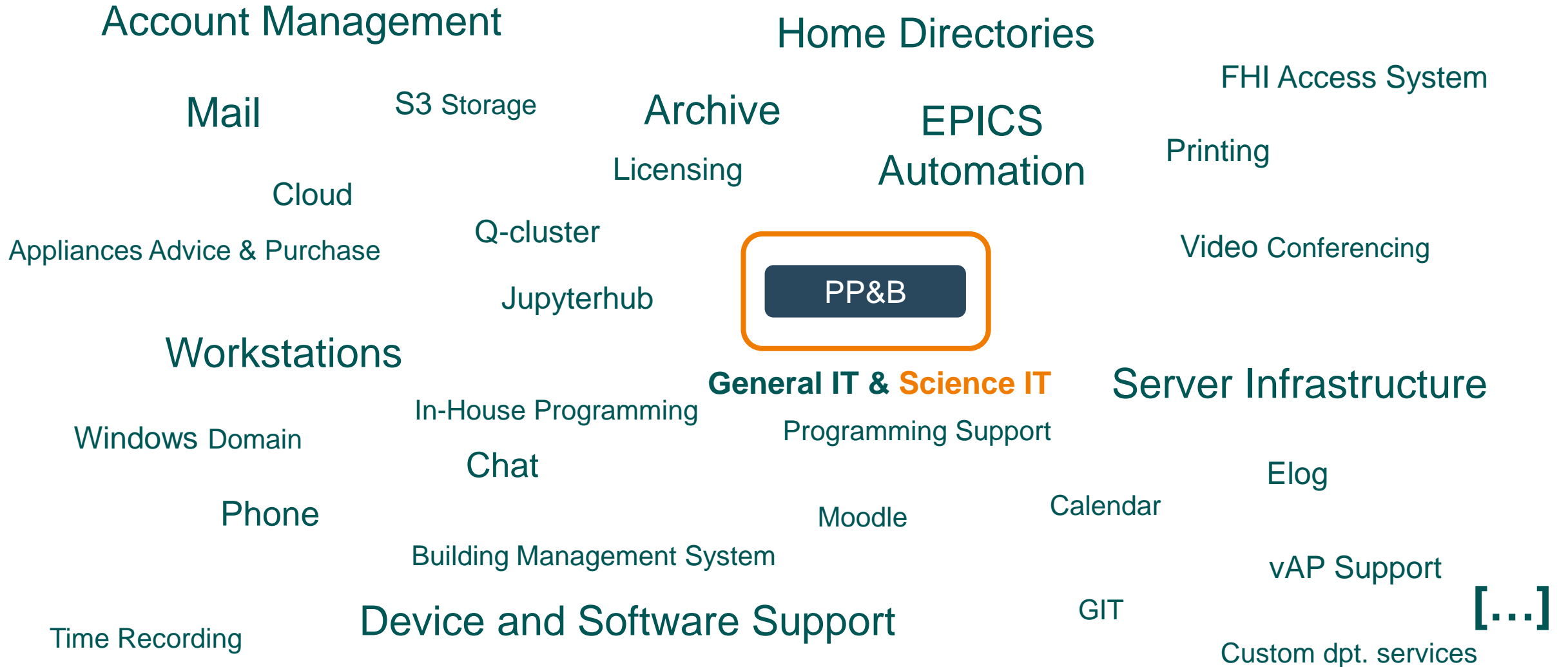


# PP&B – COMPUTER SUPPORT GROUP





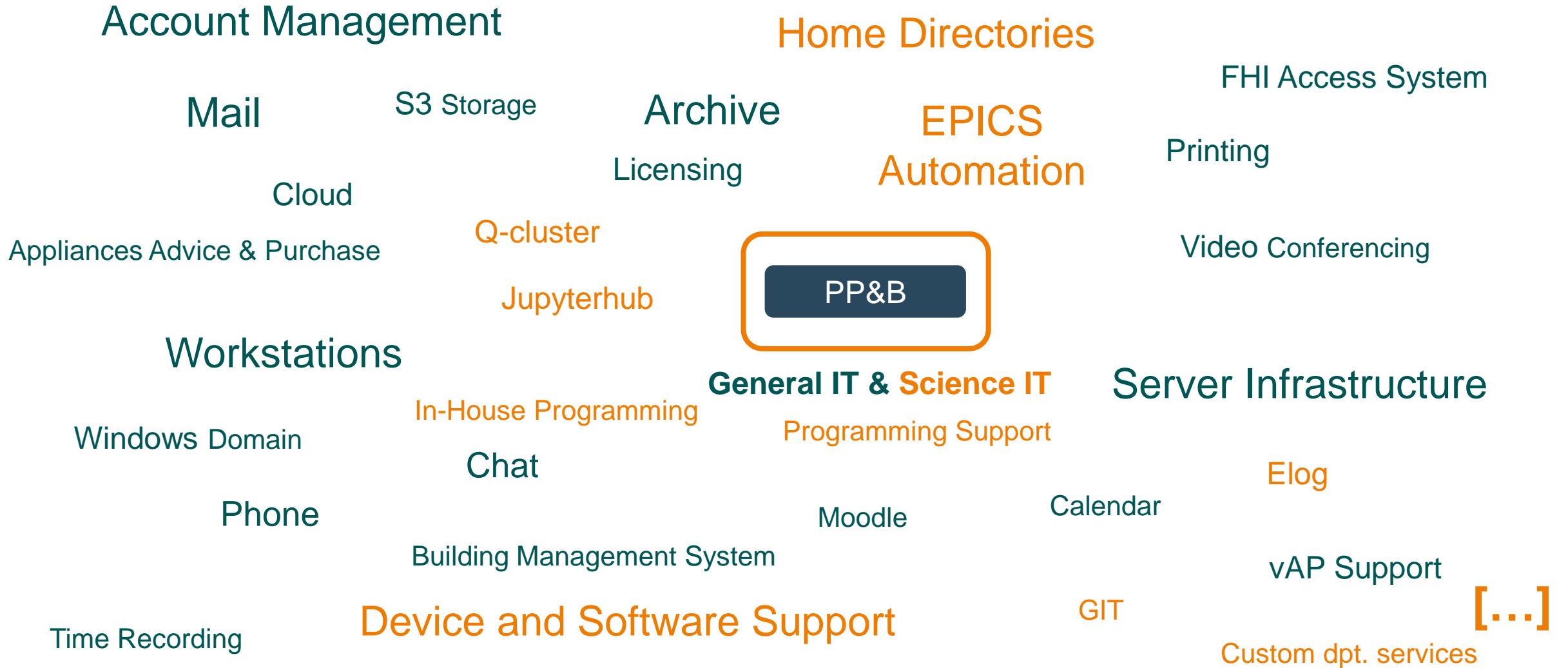
# PP&B – COMPUTER SUPPORT GROUP





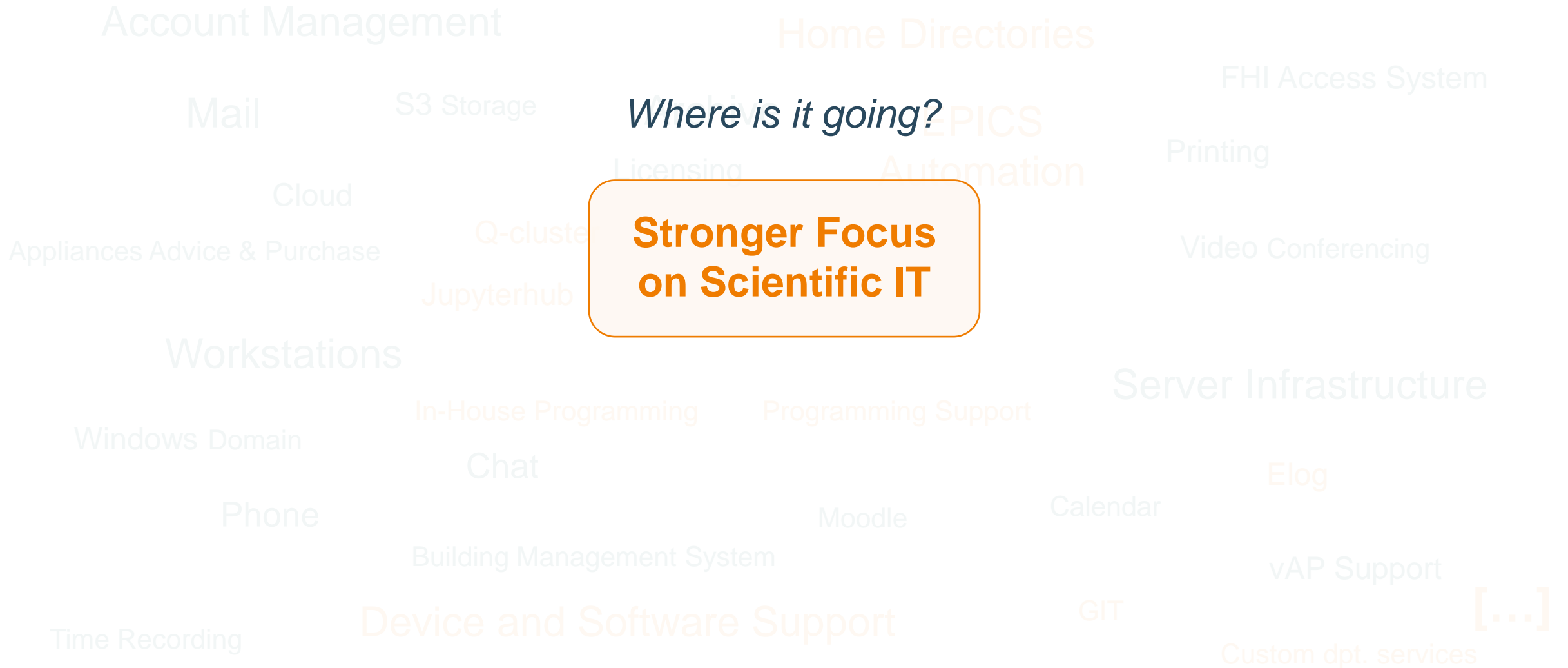


# PP&B – COMPUTER SUPPORT GROUP





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# PP&B – COMPUTER SUPPORT GROUP

**Automation**

**Automation Support**

**In-house programming**

**Move Services**

(In-house)

- *E.g. Access System, TimeRec*  
→ **Facility management**

**Stronger Focus on Scientific IT**

**Unify Services**

(or drop)

- **Single, not multiple** solutions for the same problem

**Move Services**

(External)

- *E.g. Mail, Cloud*  
→ **GWDG**
- *E.g. Cluster Hardware, JupyterHub, Storage, Virtual Servers*  
→ **MPCDF**

**Programming Support**

**Computing Support**



# PP&B – COMPUTER SUPPORT GROUP



**Sven Pokrzykowski**

FHI accounts, mail, phones  
server & Windows administration,  
licensing, IT support ...



**Heinz Junkes**

Head of PP&B,  
management,  
EPICS automation ...



**Mike Wesemann**

Storage, backup, archive system,  
server administration,  
software development



**Marco Hollemann**

Workstation infrastructure  
Windows administration & support,  
client monitoring



**Ina Richter**

FHI accounts, phones,  
door access system,  
IT support ...

*Who we are ...*



**4 new Apprentices**

*Mathematical technical software  
development, System Integration, Application  
development (→ 08.2024)*



**William Kirstaedter**

Software development,  
system integration,  
EPICS automation



**Simeon Beinlich**

HPC systems,  
scientific computing,  
scientific programming



**Falk Rosenhahn**

Elab-IT / PP&B



**CHALLENGES IN SCIENTIFIC IT**

**&**

**POSSIBLE WAYS TO TACKLE THESE**



# CHALLENGES IN SCIENTIFIC IT – MORE COMPLEXITY

More data

More complex data

More complex analyses

*... More IT ...*

More complex setups

More requirements



# CHALLENGES IN SCIENTIFIC IT - MORE REQUIREMENTS

**Reproducibility  
& Documentation**

**Data Management**  
*What did I store and where?*

- Data Security**
- *Hardware failures*
  - *Cyberattacks (HZB, BHT, ...)*
  - *Human errors ...*

**Data Provenance**  
*What happened to the sample  
until it was measured?*

*How to tackle this?*

**Setup Complexity  
& Stability**

**Accessibility &  
Findability**  
*Internally & externally*

**Reusability & Uniformity**  
*Data & procedures!*

**Independence from  
vendors**

**AI?!**





# CHALLENGES IN SCIENTIFIC IT - MORE REQUIREMENTS

**Reproducibility  
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**INFRASTRUCTURE  
AUTOMATION  
COLLABORATION**

**Setup Complexity  
& Stability**

**Accessibility &  
Findability**

*Internally & externally*

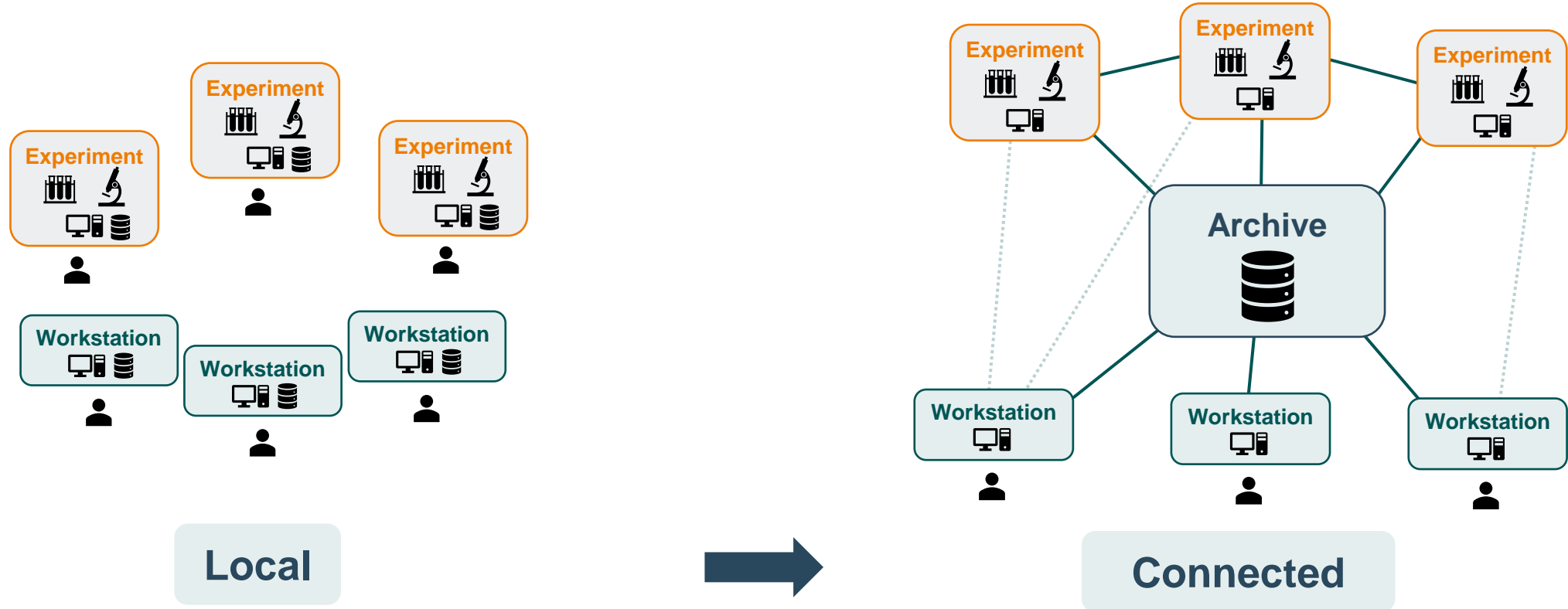
**Reusability & Uniformity**  
*Data & procedures!*

**Independence from  
vendors**

**AI?!**



# INFRASTRUCTURE, AUTOMATION, & COLLABORATION



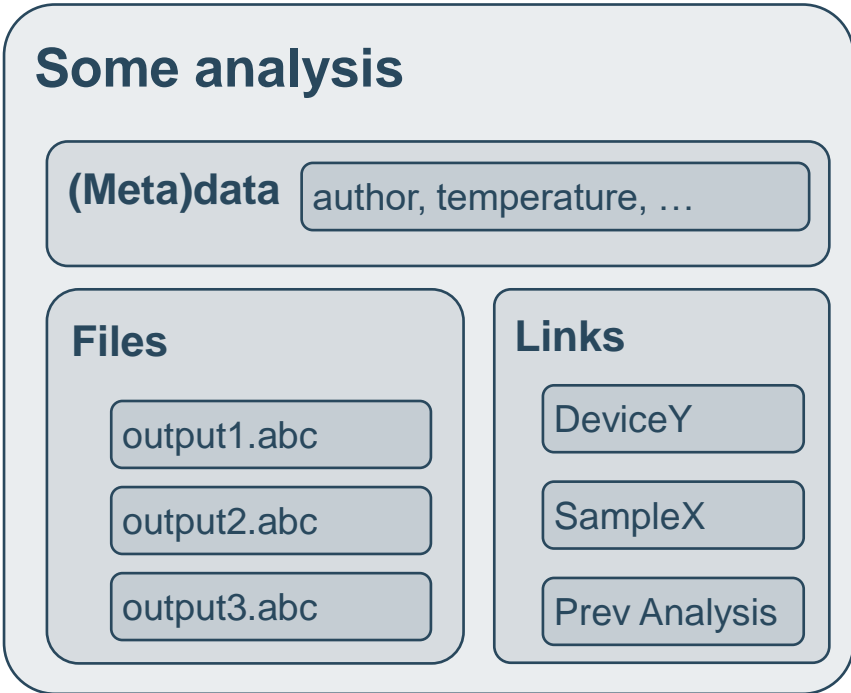
**Local**  
Single Person  
*Repetitive manual workflow*

**Connected**  
Group  
*Streamlined automatized workflow*

- |              |                 |                     |                                     |
|--------------|-----------------|---------------------|-------------------------------------|
| <b>GOALS</b> | • Findable data | • Reproducible data | • Streamlined & reusable procedures |
|              | • Uniform data  | • Documented data   |                                     |
|              | • Secure data   | • Data provenance   |                                     |



# INFRASTRUCTURE – THE FHI ARCHIVE



Data Management

Data Security

Accessibility & Findability

Reusability & Uniformity

Reproducibility & Documentation

Data Provenance

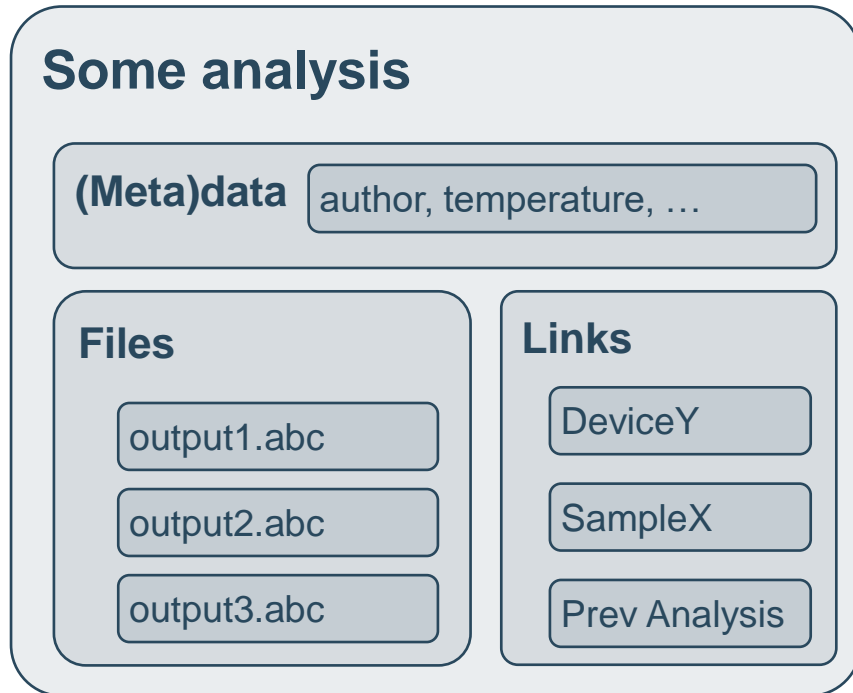
Setup Complexity & Stability

Independence from vendors

AI?!

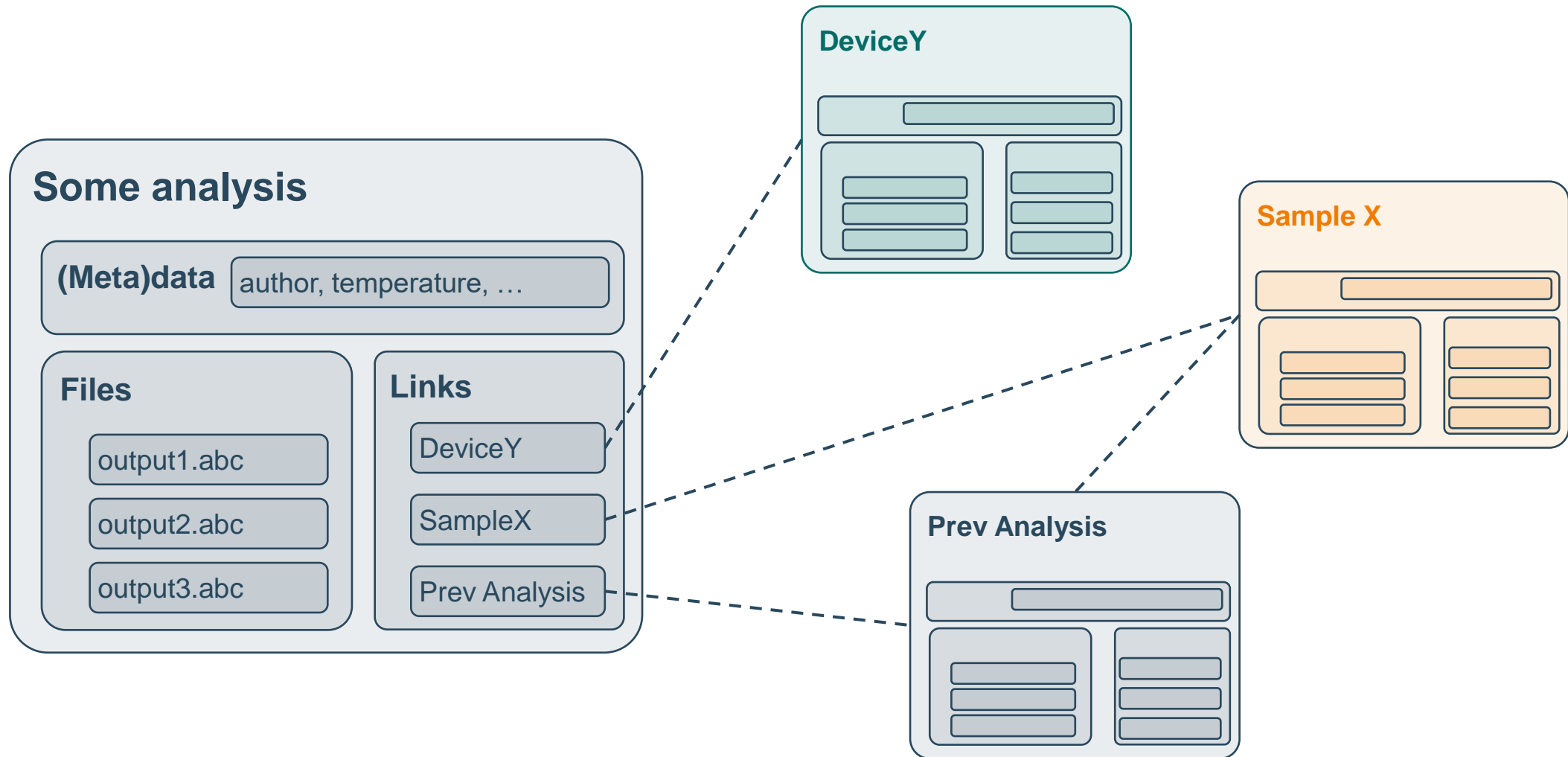


# INFRASTRUCTURE – THE FHI ARCHIVE



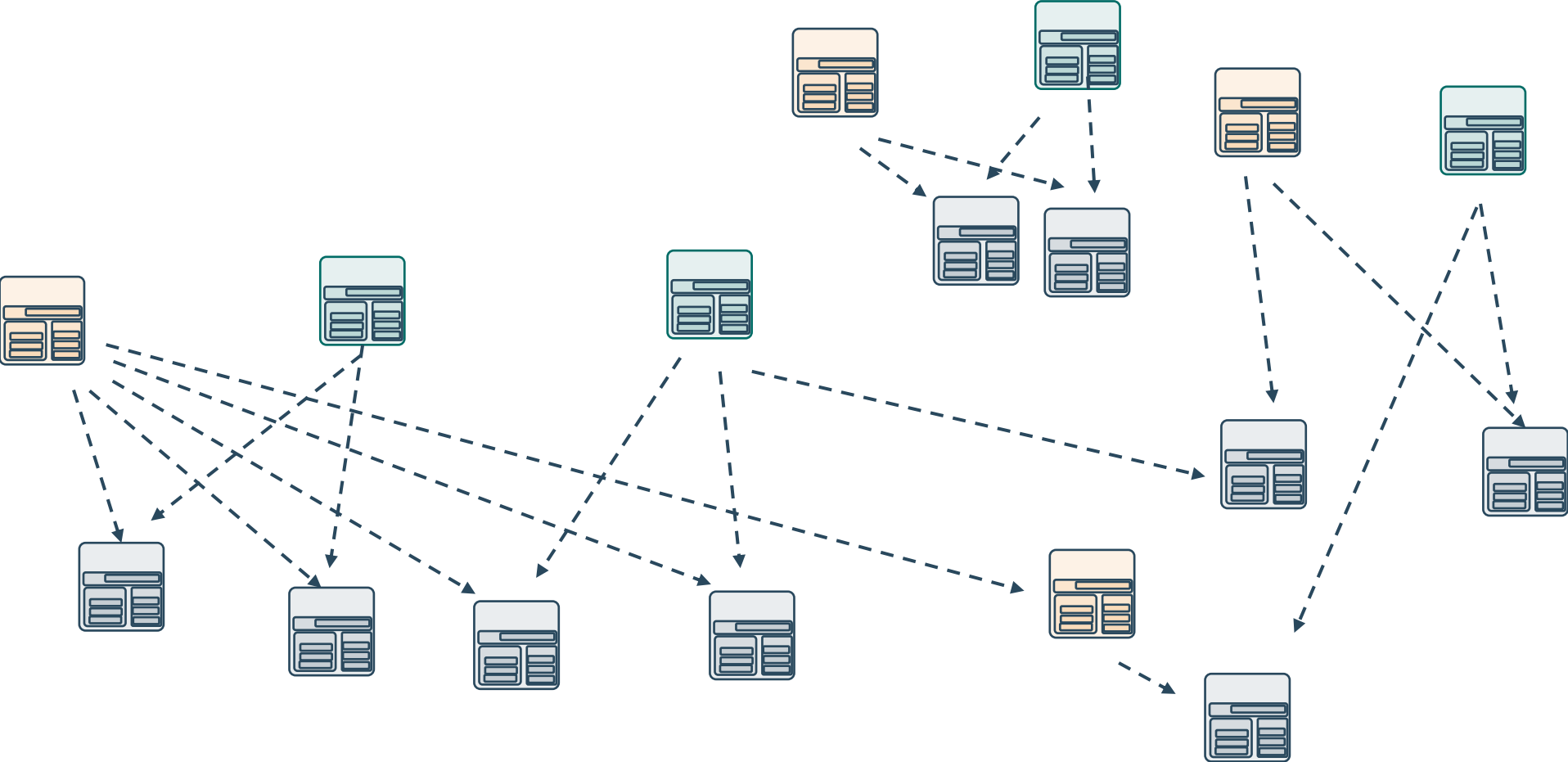


# INFRASTRUCTURE – THE FHI ARCHIVE





# INFRASTRUCTURE – THE FHI ARCHIVE

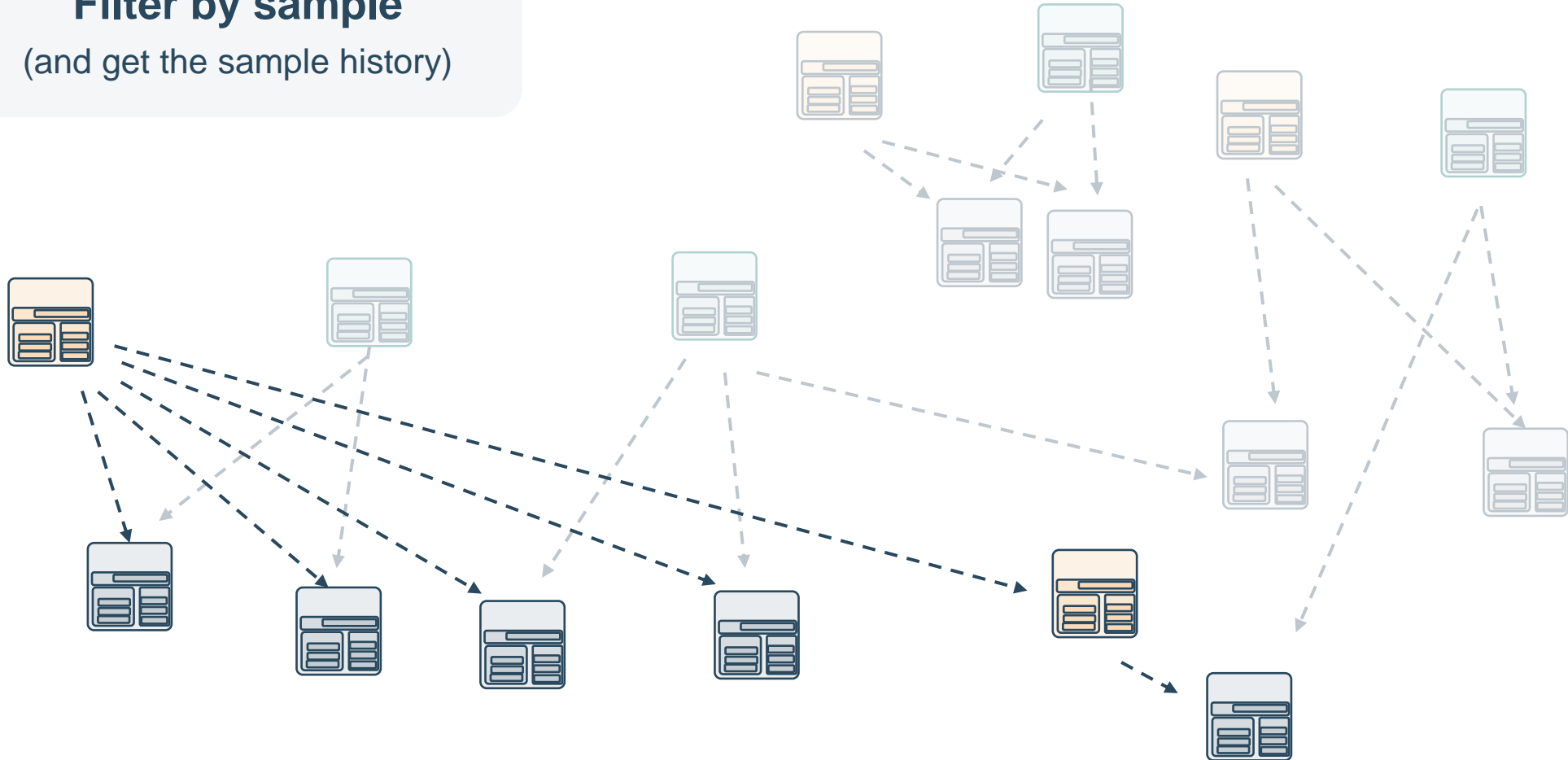




# INFRASTRUCTURE – THE FHI ARCHIVE



**Filter by sample**  
(and get the sample history)

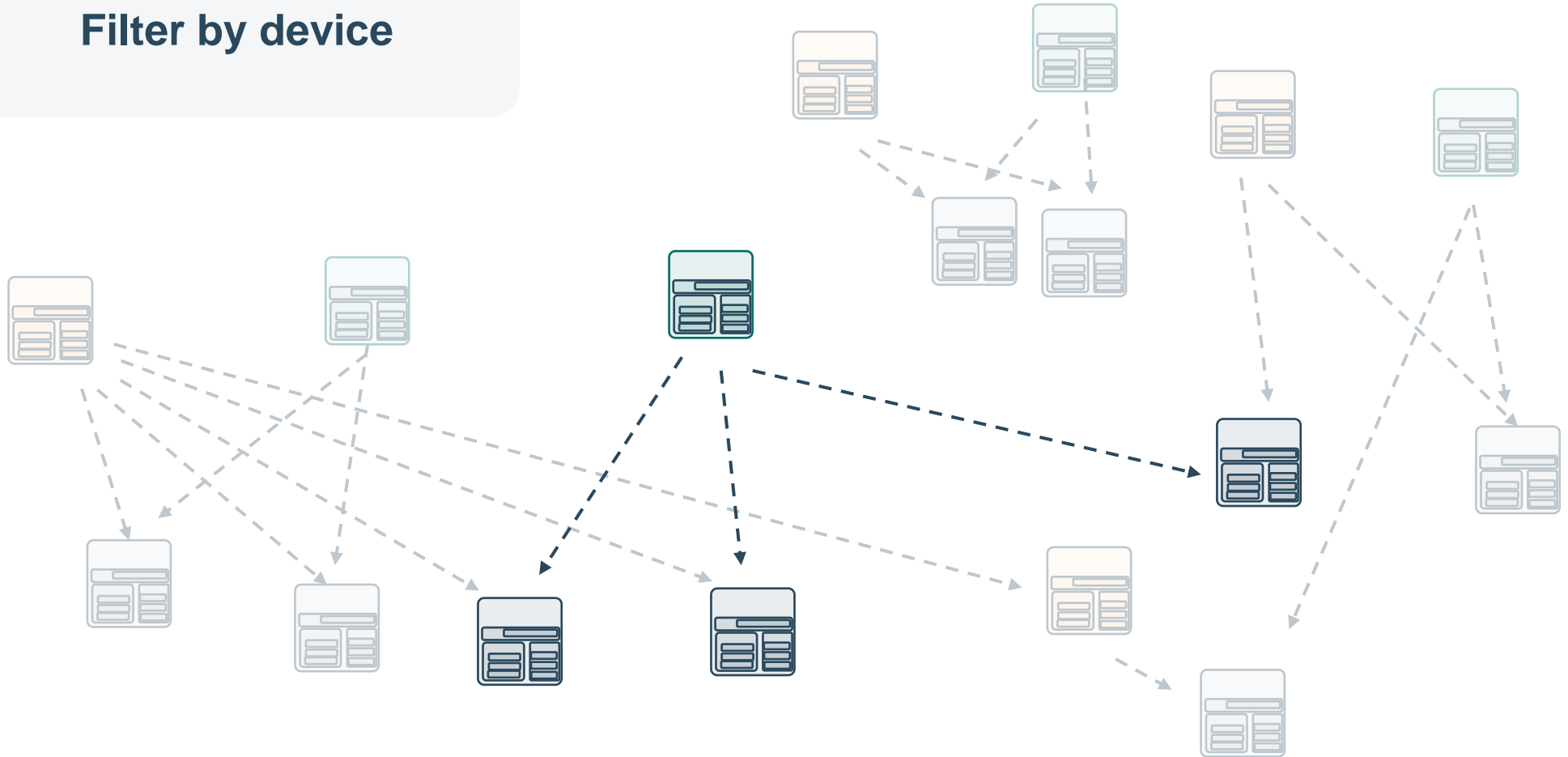




# INFRASTRUCTURE – THE FHI ARCHIVE



**Filter by device**



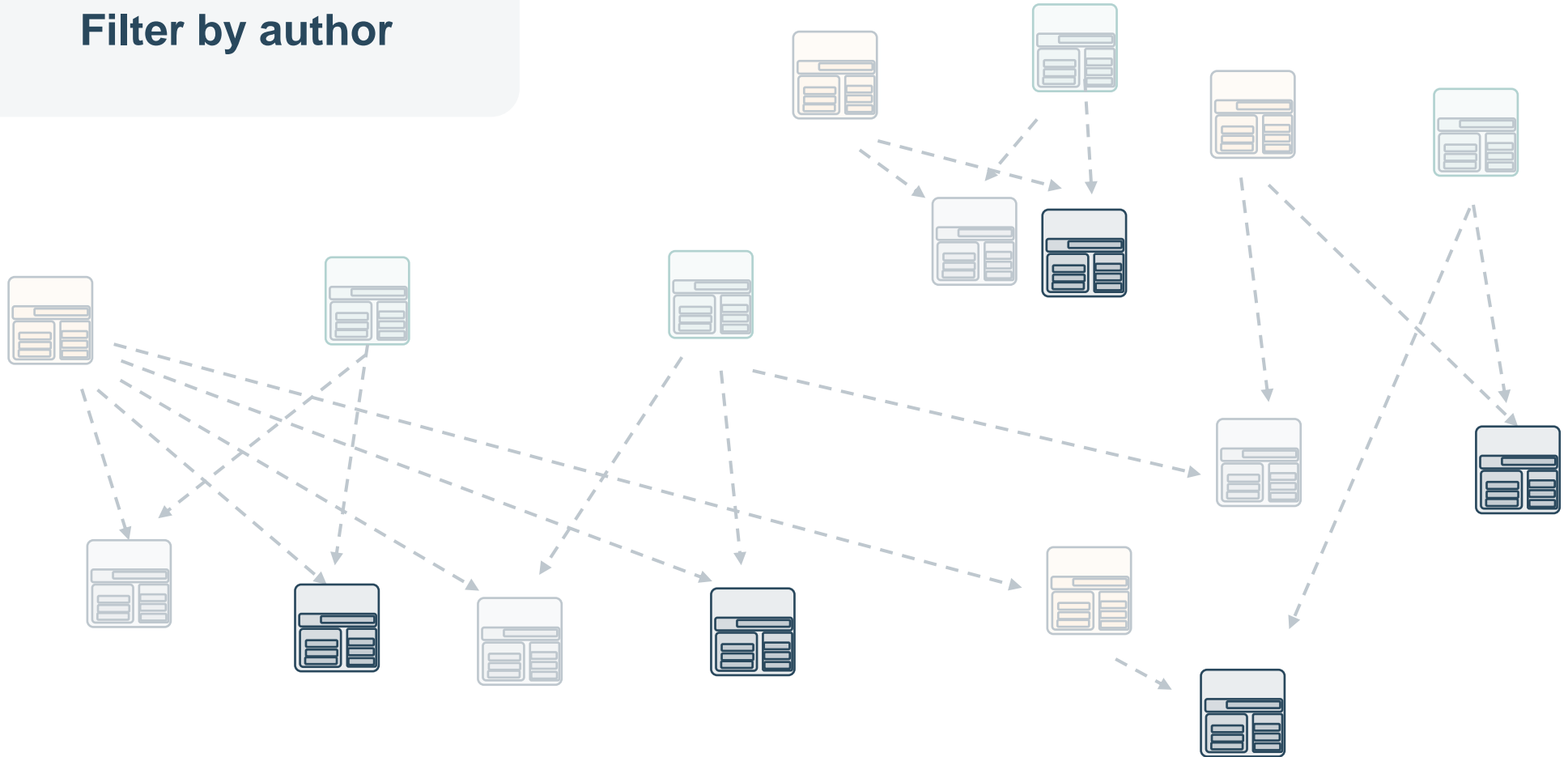




# INFRASTRUCTURE – THE FHI ARCHIVE

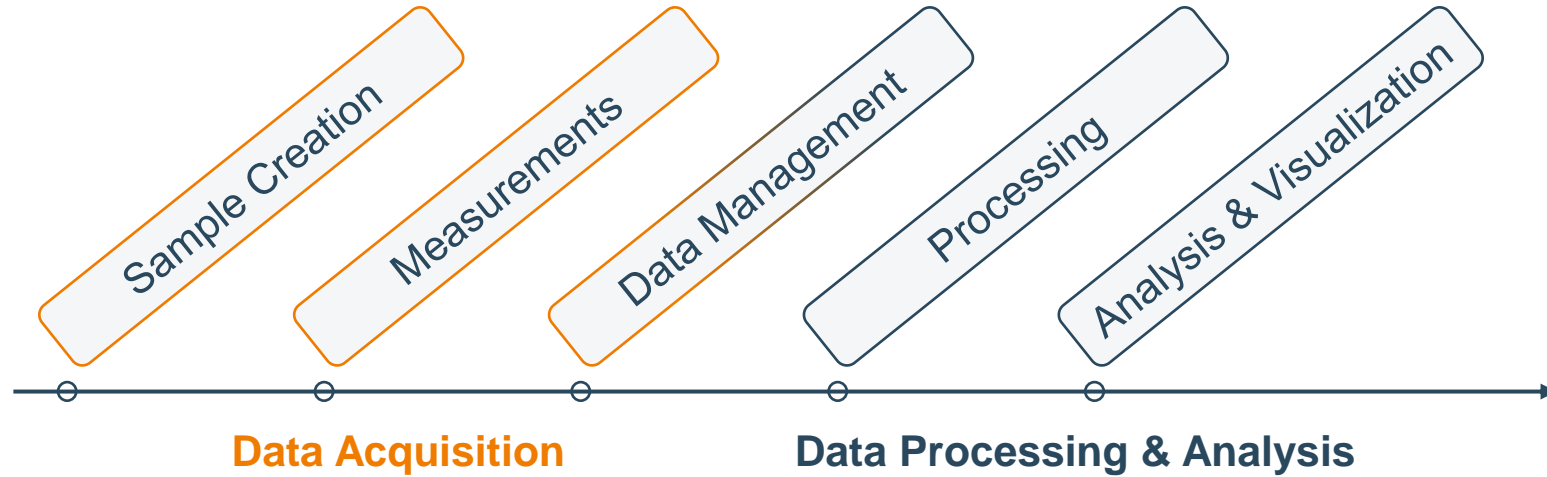
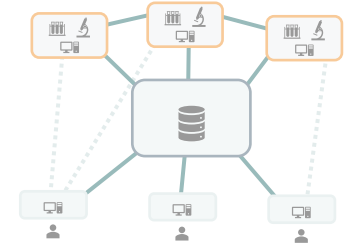
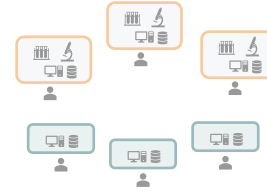
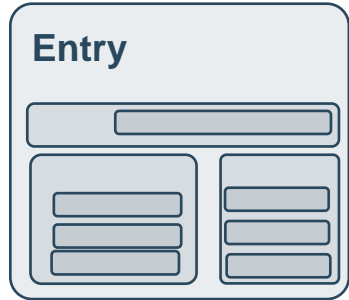


**Filter by author**





# CHALLENGES IN SCIENTIFIC IT

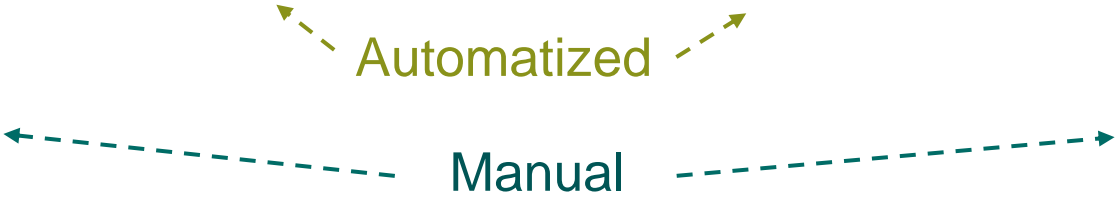


**EPICS Automation**

**Scripted Analyses**  
(Python, Archive, ...)

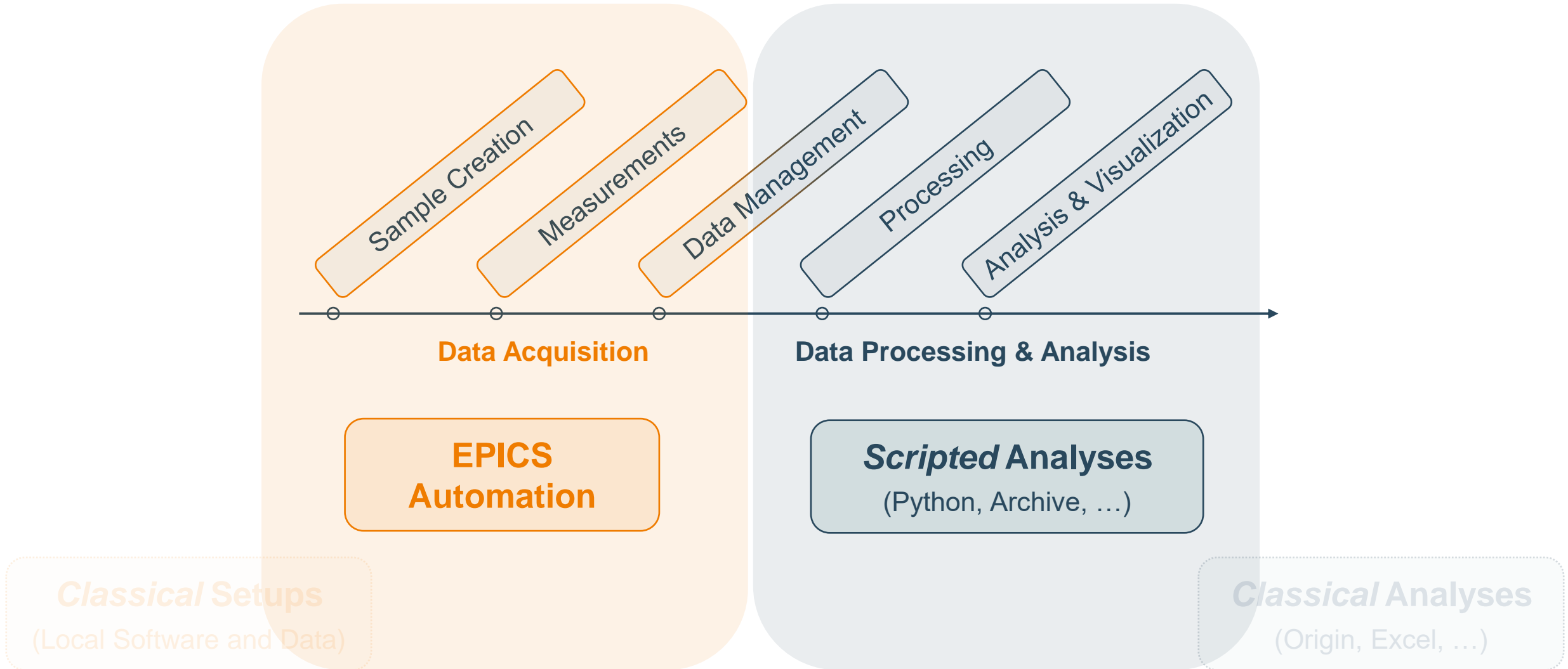
**Classical Setups**  
(Local Software and Data)

**Classical Analyses**  
(Origin, Excel, ...)





# A FULLY AUTOMATIZED EXAMPLE – HABER REACTOR (AC)

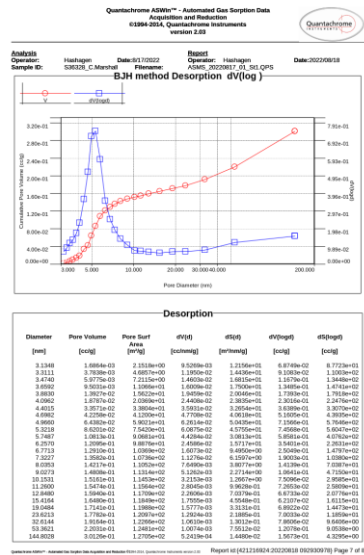
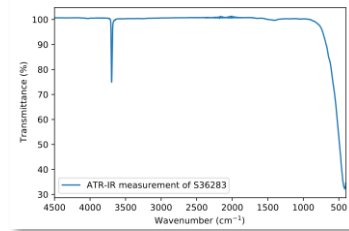




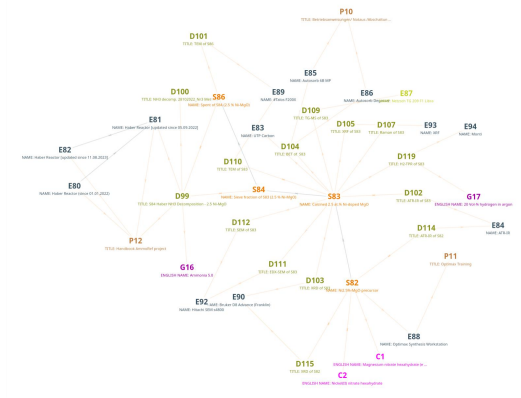
# A FULLY AUTOMATIZED EXAMPLE – HABER REACTOR (AC)

## Automated:

- Experimental control (EPICS)
- Data collection & linking (Archive)
- Data processing (Python)
- Plotting / Reporting (Python)



| Id   | Project | File                          | Time                | Comment | Size    | Action |
|------|---------|-------------------------------|---------------------|---------|---------|--------|
| 1011 | DEFAULT | ATR-IR measurement of S82.csv | 2024-05-27 16:41:09 |         | 60.1 kb |        |
| 1012 | DEFAULT | ATR-IR Spectrum of S82.pdf    | 2024-05-27 16:41:09 |         | 21.2 kb |        |



ChemRxiv®

How To Submit Browse About News

Catalysis

## Advancing Catalysis Research through FAIR Data Principles Implemented in a Local Data Infrastructure - A Case Study of an Automated Test Reactor

10 June 2024, Version 2

Working Paper

Abdulrhan Moshantaf, Michael Wesemann, Simeon Beinlich, Heinz Junkes, Julia Schumann, Baris Alkan, Pierre Kube, Clara Patricia Marshall, Nils Pfister, Annette Trunschke

Show author details

A. Trunschke et al. *ChemRxiv* (2024)

Demo Archive (Open Access)  
haber.archive.fhi.mpg.de

| Id   | Project | Type                                     | Author                                | Action |
|------|---------|--|---------------------------------------|--------|
| 1194 | DEFAULT | Pike GluATR, Diamant ATR                 | Pierre Kube                           |        |
| 1193 | DEFAULT | Presswerkzeug                            | Pike Technologies                     |        |
| 1192 | DEFAULT | laboratory press                         | FLUXANA GmbH                          |        |
| 1191 | DEFAULT | balance                                  | Maassen                               |        |
| 1190 | DEFAULT | Vulcan Fusion Machine                    | Kern                                  |        |
| 1189 | DEFAULT | X-ray fluorescence spectrometer SB-TIGER | HD Elektronik und Elektrotechnik GmbH |        |
| 1188 | DEFAULT | Raman spectroscopy                       | BRUKER AXS                            |        |
| 1187 | DEFAULT | Germanium accessory                      | Tempo G                               |        |
| 1186 | DEFAULT | PC100                                    | WTEC                                  |        |
|      |         |  | Perkin Elmer                          |        |
|      |         |  | Perkin Simer                          |        |



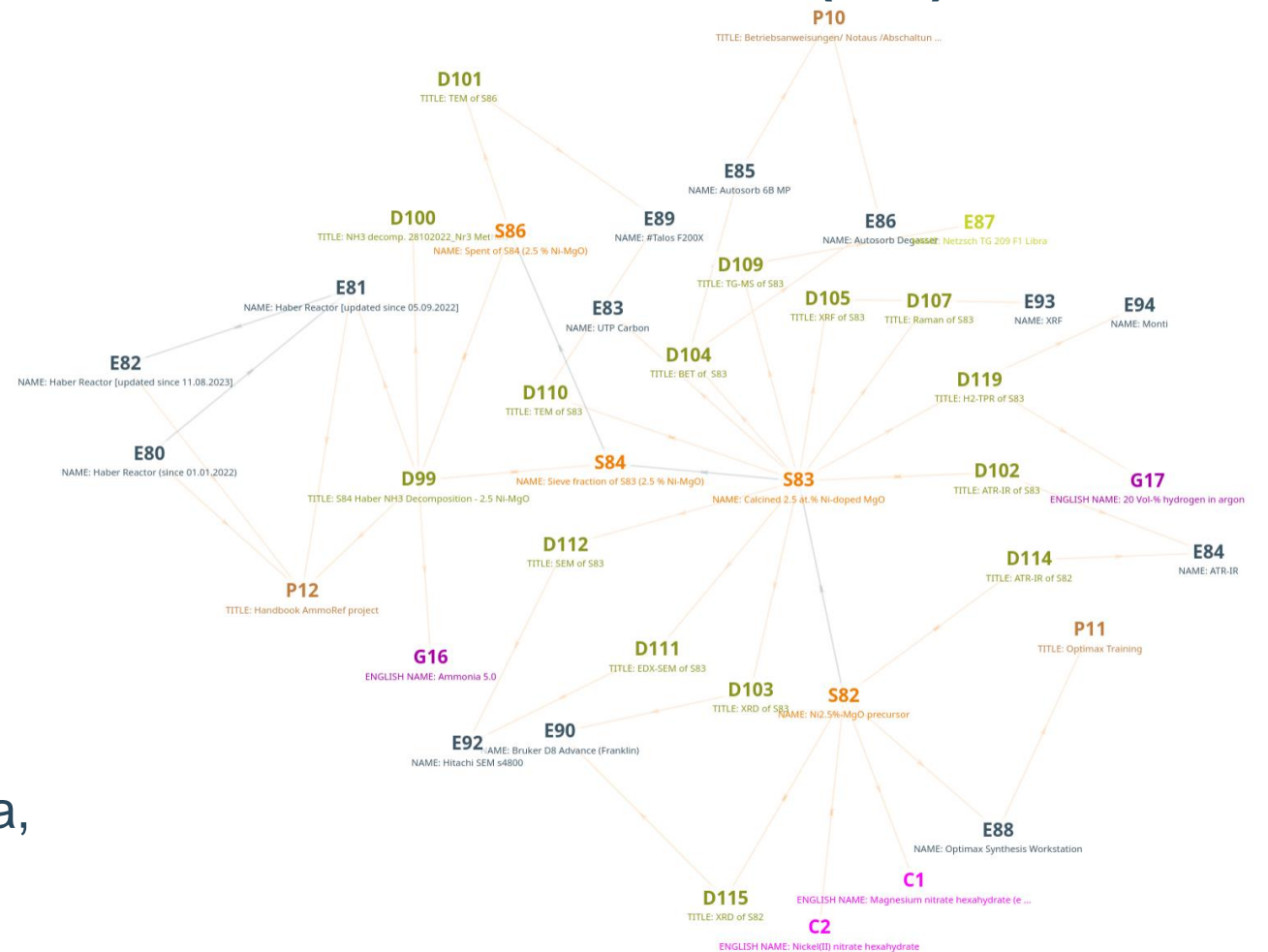
# A FULLY AUTOMATIZED EXAMPLE – HABER REACTOR (AC)

## Automatized:

- Experimental control (EPICS)
- Data collection & linking (Archive)
- Data processing (Python)
- Plotting / Reporting (Python)

## Provenance from start to finish:

- Sample creation, modification & characterization
- Measurement parameters, raw data, processing, plotting & reporting.
- Access to other parameters (room temperature, humidity, ...)



**Demo Visualizer (Open Access)**  
[visualizer.fhi.mpg.de/haber](https://visualizer.fhi.mpg.de/haber)



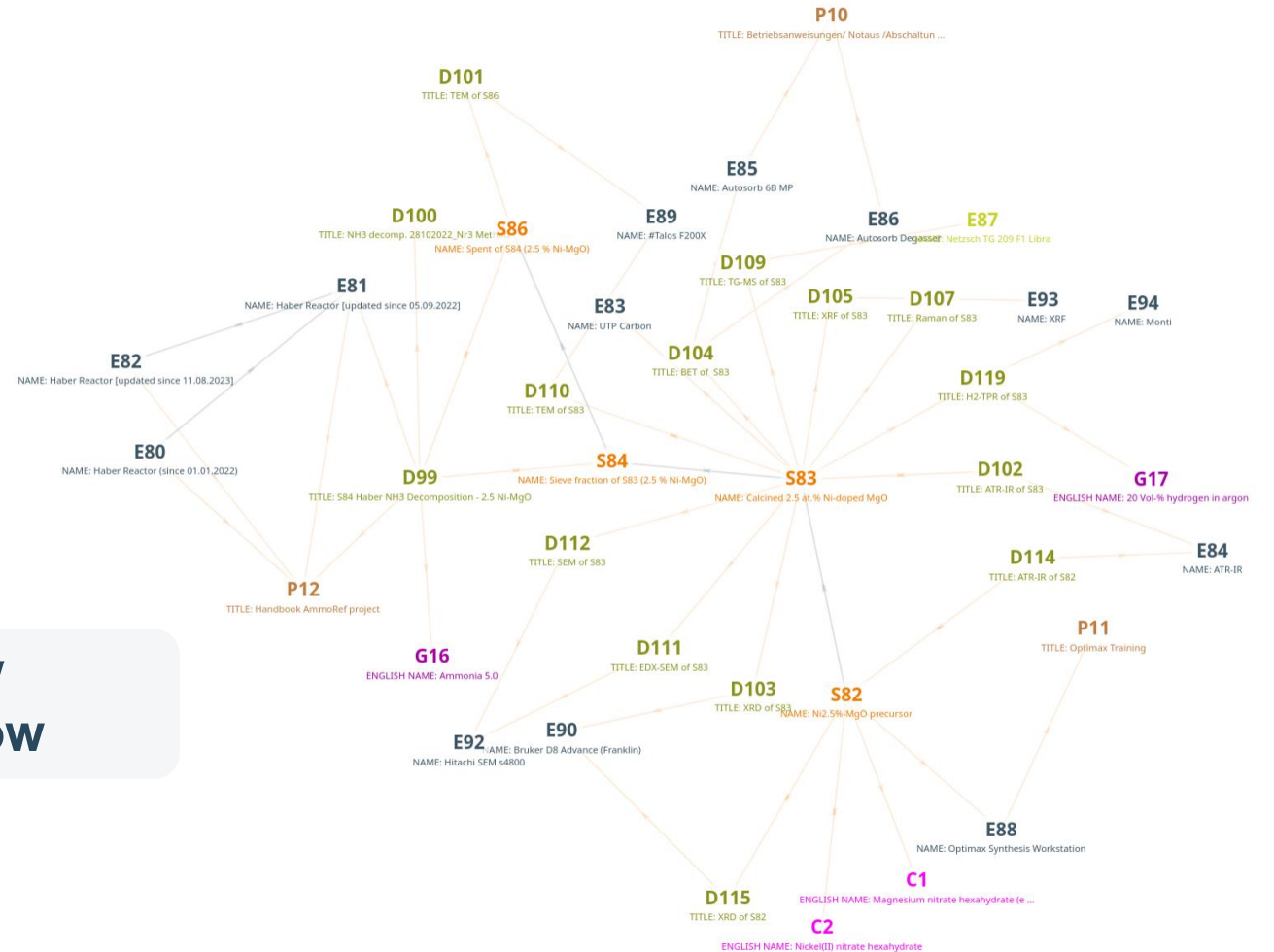
# EXAMPLE FOR TAILORED SERVICES: ARCHIVE VISUALIZER

## Visualization of connected Archive Entries as a Network Graph

Explore Entries

Search Connections

Follow Data Flow

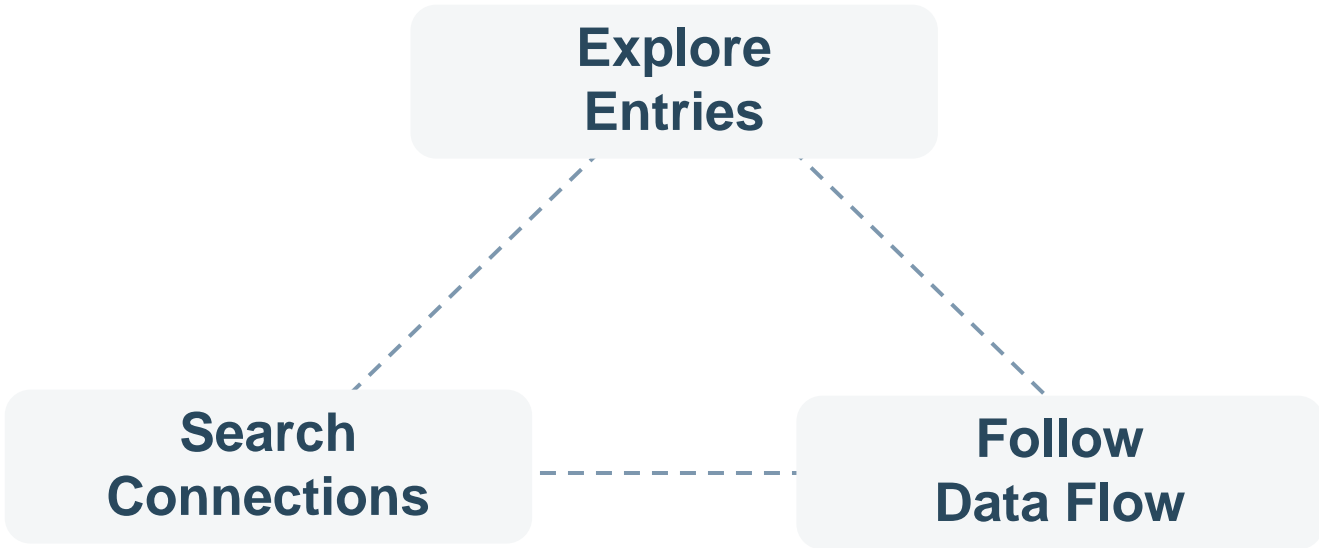


**Demo Visualizer (Open Access)**  
[visualizer.fhi.mpg.de/haber](https://visualizer.fhi.mpg.de/haber)



# EXAMPLE FOR TAILORED SERVICES: ARCHIVE VISUALIZER

## Visualization of connected Archive Entries as a Network Graph



**Demo Visualizer (Open Access)**  
[visualizer.fhi.mpg.de/haber](https://visualizer.fhi.mpg.de/haber)

| Id  | Project |  | Action                |
|-----|---------|--|-----------------------|
| D99 | DEFAULT | S84 Haber NH3 Decomposition - 2.5 Ni-MgO | B. Alkan, C. Marshall |
| S86 | DEFAULT | Spent of S84 (2.5 % Ni-MgO)              | B. Alkan, C. Marshall |
| S84 | DEFAULT | Sieve fraction of S83 (2.5 % Ni-MgO)     | M. Ertegi             |



# EXAMPLE FOR TAILORED SERVICES: ARCHIVE VISUALIZER

## Institute-wide solutions

Developed for one department










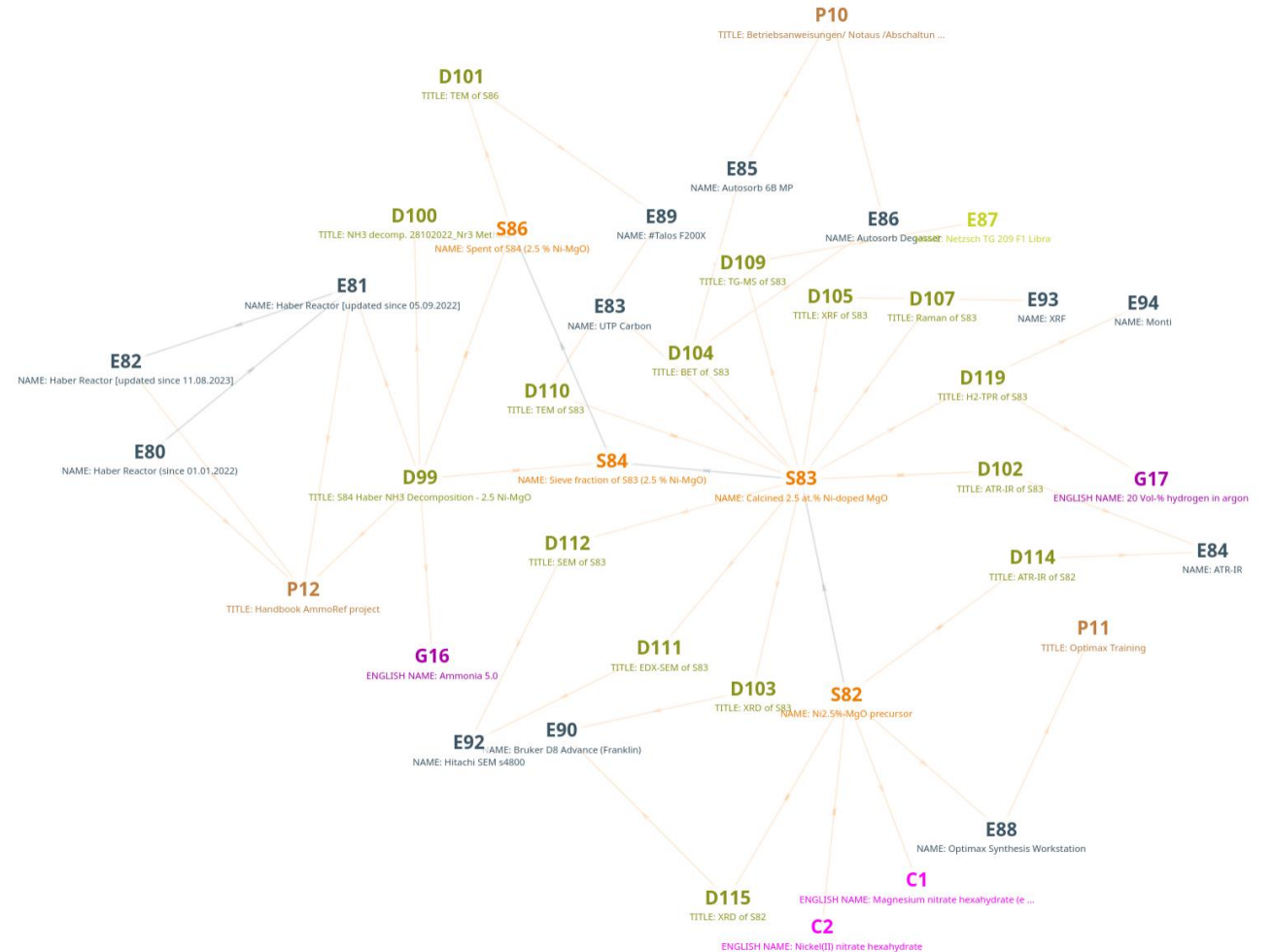
Useable by all departments

AC/CATLAB Archive v1.0.197

User: beinlich Role: admin Type: local

### Metadata

| Action               |        |
|----------------------|---|
| <b>Id</b>            | D63096  |
| <b>User</b>          | haberreactor  |
| <b>Project</b>       | DEFAULT   |
| <b>Access</b>        | project   |
| <b>Open Access</b>   |   |
| <b>Edit History</b>  | <a href="#">SHOW</a>  |
| <b>Date Created</b>  | 2024-07-07 13:07:52   |
| <b>Date Modified</b> | 2024-07-07 13:07:53   |

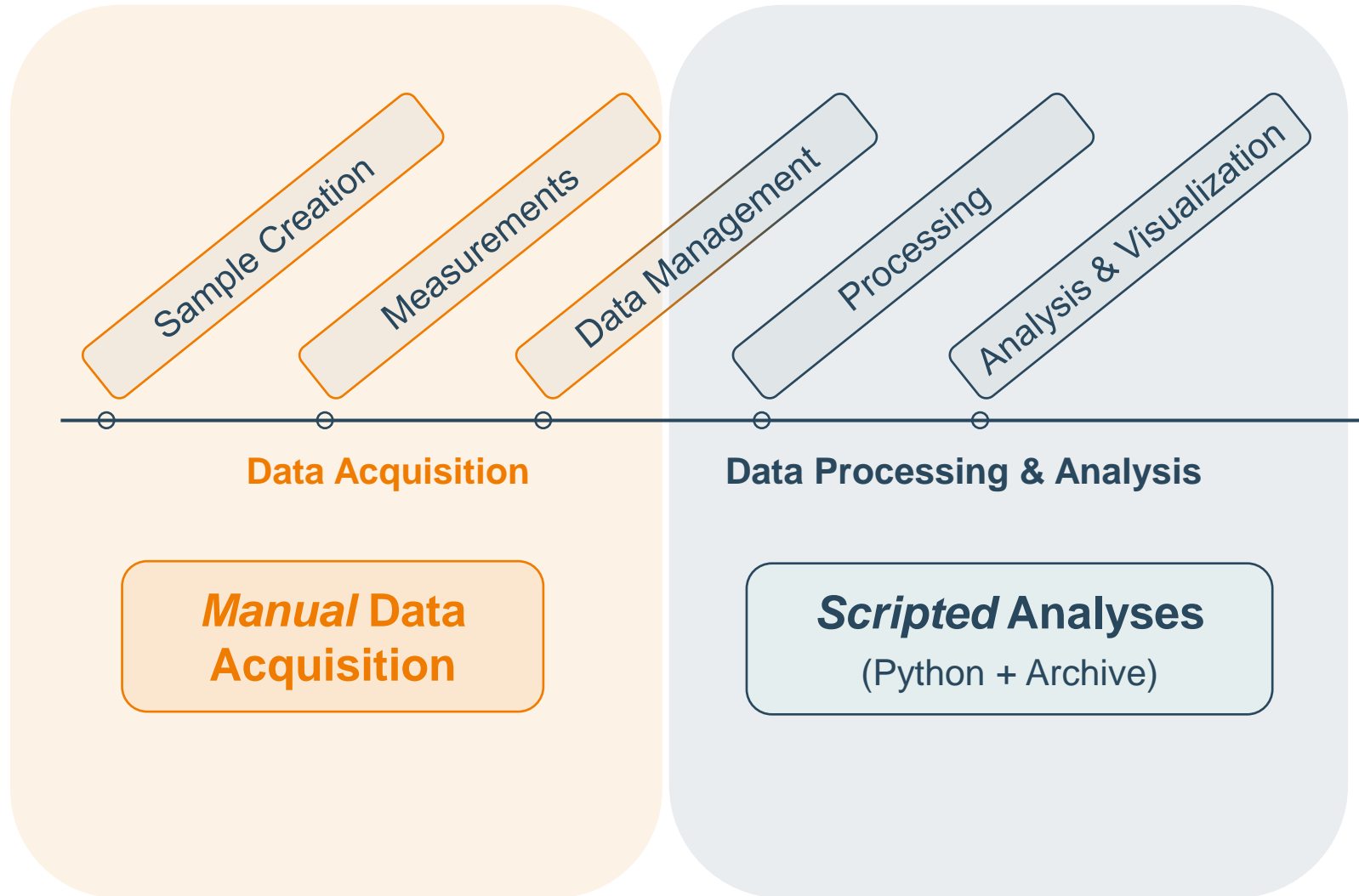


Demo Visualizer (Open Access)  
[visualizer.fhi.mpg.de/haber](http://visualizer.fhi.mpg.de/haber)



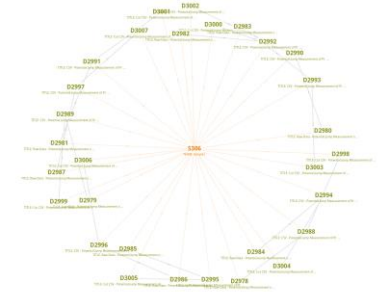
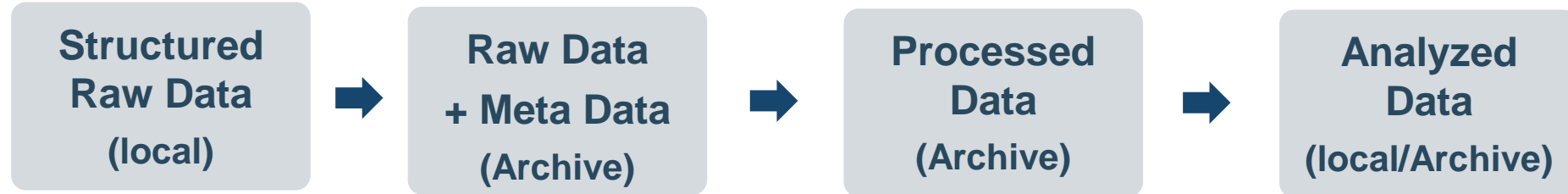


# A HALF-AUTOMATIZED EXAMPLE





# A HALF-AUTOMATIZED EXAMPLE



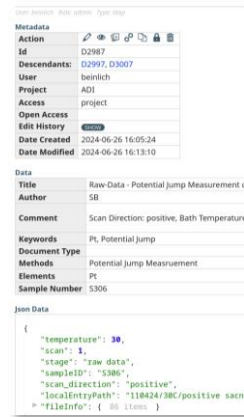
```

sample-1
├── 10C
│   ├── 1V
│   │   ├── run-1.dat
│   │   ├── run-2.dat
│   │   ├── run-3.dat
│   │   ├── run-4.dat
│   │   └── run-5.dat
│   ├── 2V
│   │   ├── run-1.dat
│   │   ├── run-2.dat
│   │   ├── run-3.dat
│   │   ├── run-4.dat
│   │   └── run-5.dat
│   ├── 3V
│   │   ├── run-1.dat
│   │   ├── run-2.dat
│   │   ├── run-3.dat
│   │   ├── run-4.dat
│   │   └── run-5.dat
│   └── 4V
│       ├── run-1.dat
│       ├── run-2.dat
│       └── run-3.dat
  
```

> 1000 Files

Metadata from:

- folder structure
- data header
- manually entered'



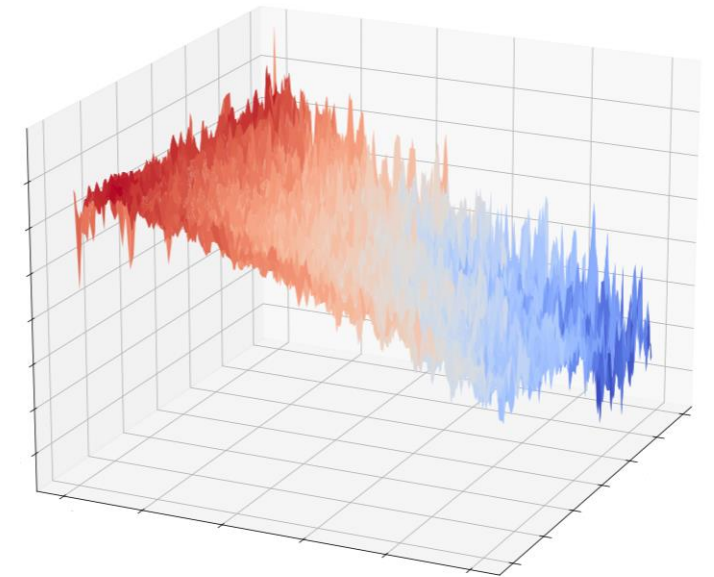
```

"temperature": 30,
"scan": 1,
"sampleID": "S307",
"scan_direction": "positive",
"step_number": "1"
  
```



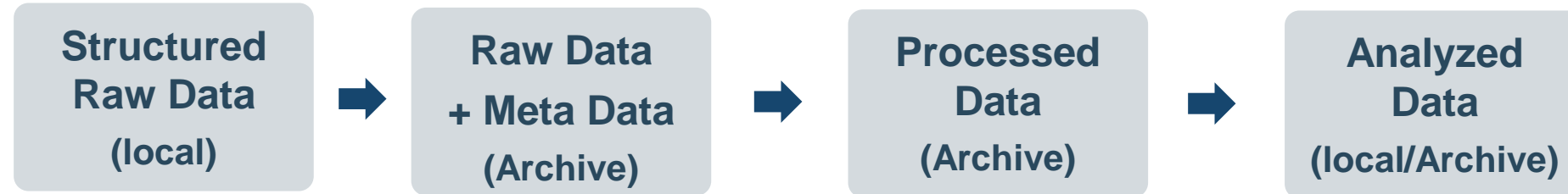
```

"VSTEP1": 0.1,
"VSTEP2": 0.15,
"VSTEP1": 0.15,
"VSTEP2": 0.15,
"SAMPLETIME": 0.0000033334,
"start_index": 0,
"end_index": 90006,
  
```





# A HALF-AUTOMATIZED EXAMPLE



## Automatize repetitive tasks

- Data collection
- Data processing
- Analysis
- Plotting

## Python: *simple & powerful*

- Local workstation
- JupyterHub
- HPC

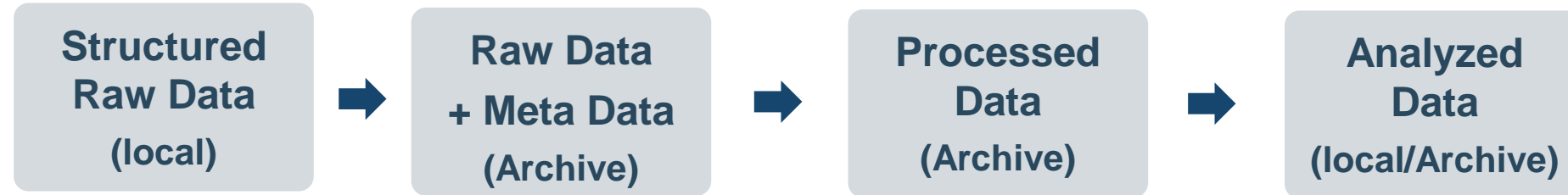
### PYTHON

| IPY-Notebooks  | Modules  |
|--|--|
| <ul style="list-style-type: none"><li>• raw_data.ipynb</li><li>• (pre-)processing.ipynb</li><li>• analysis.ipynb</li></ul> | <ul style="list-style-type: none"><li>• Archive Rest API</li><li>• Archive Python API</li><li>• Archive Python DAO (Database Access Object)</li><li>• Archive Dataframe Extension (Pandas)</li></ul> |

*Here: provided ready to run by PP&B*



# A HALF-AUTOMATIZED EXAMPLE



## But I don't know Programming?

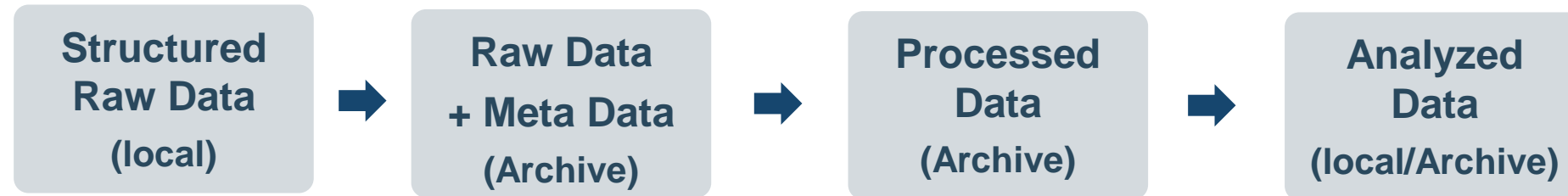
- Use pre-made scripts/notebooks from:  
    **Colleagues, PP&B, Theory?, ...**
- Modify existing notebooks
- Then maybe: Write your own!

### PYTHON

| IPY-Notebooks   | Modules  |
|---|--|
| <ul style="list-style-type: none"><li>• <code>raw_data.ipynb</code></li><li>• <code>(pre-)processing.ipynb</code></li><li>• <code>analysis.ipynb</code></li></ul> <p><i>Here: provided ready to run by PP&amp;B</i></p> | <ul style="list-style-type: none"><li>• <b>Archive Rest API</b></li><li>• <b>Archive Python API</b></li><li>• <b>Archive Python DAO</b> (Database Access Object)</li><li>• <b>Archive Dataframe Extension</b> (Pandas)</li></ul> |



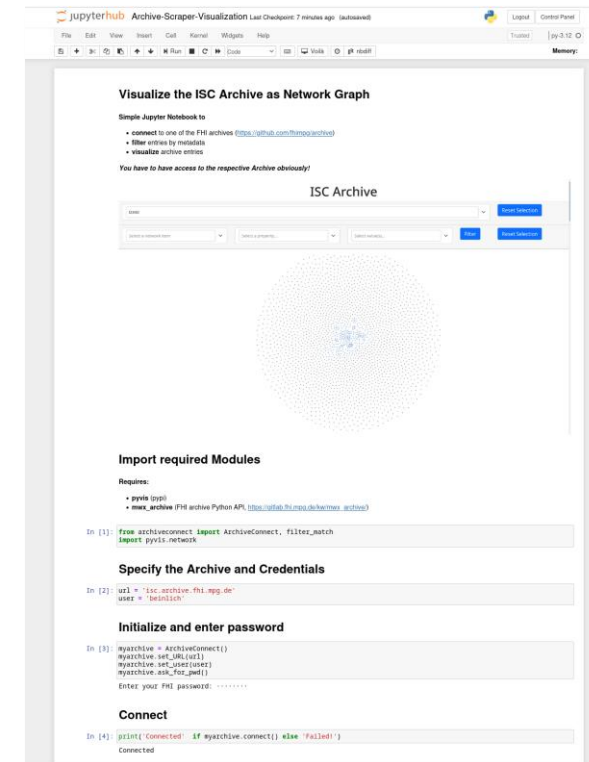
# A HALF-AUTOMATIZED EXAMPLE



## But I don't know Programming?

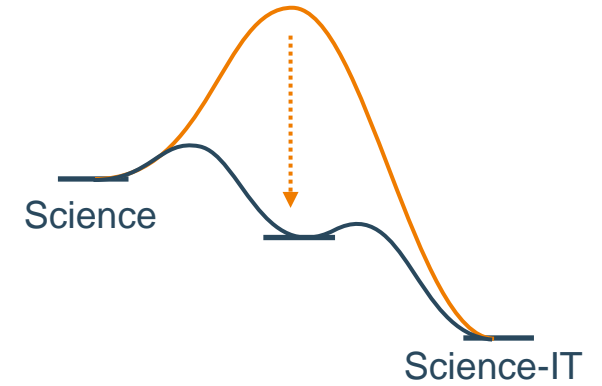
- Use pre-made scripts/notebooks from:  
    **Colleagues, PP&B, Theory?, ...**
- Modify existing notebooks
- Then maybe: Write your own!

**Ask for ready-made Notebooks on JupyterHub as a start!**





# PYTHON SCRIPTING AND SMALL SERVICES



**Help with programming**

- Python
- Other

**Advice on how to tackle IT problems**

**What the PP&B can do for you**

**Help with / provide small services**

- Jupyter Notebooks
- Python modules
- Python scripts
- Small services

**Help with existing services**

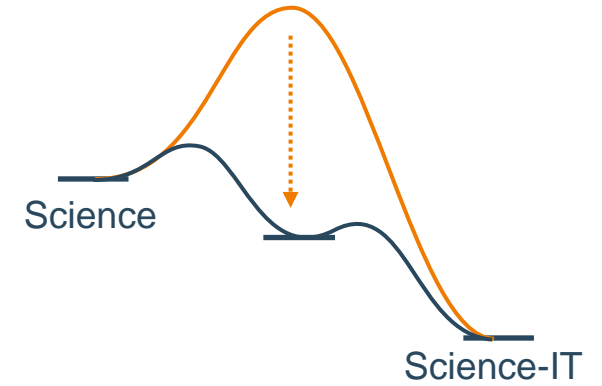
- Archive
- Cluster
- Storage
- JupyterHub
- EPICS
- ...

**Help with script sharing**

- GIT



# PYTHON SCRIPTING AND SMALL SERVICES



***Help with programming***

- Python
- Other

***Advice on how to tackle IT problems***

**What the PP&B can do for you**

***Help with / provide small services***

- Jupyter Notebooks
- Python modules
- Python scripts
- Small services

***Help with existing services***

- Archive
- Cluster
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- EPICS
- ...

***Help with script sharing***

- GIT



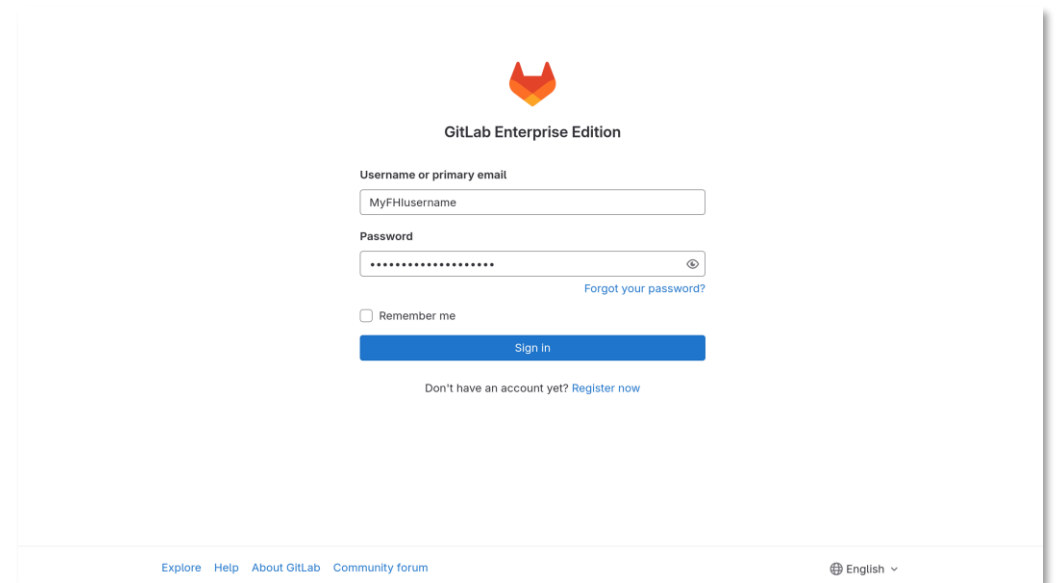
# SHARING & COLLECTING ANALYSIS PROCEDURES - GIT

**GitLab**  
=  
**Collaboration & Versioning Tool**

*Knowledge is useless if you don't share it.*

## Use Git for:

- collecting analysis procedures...
- sharing...
- improving...
- documenting (Git Wikis!)



**FHI GitLab**  
<https://gitlab.fhi.mpg.de>  
*(register first)*





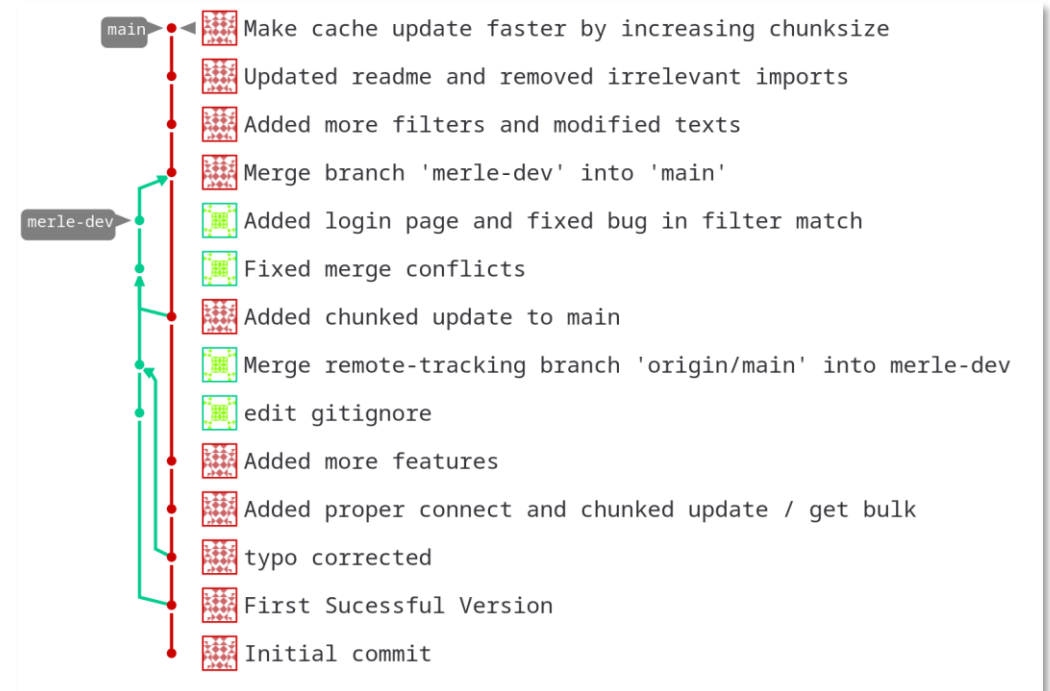
# SHARING & COLLECTING ANALYSIS PROCEDURES - GIT

**GitLab**  
=  
**Collaboration & Versioning Tool**

**Starting to use Git can be troublesome..**

- Need a kickstart?
- Got lost in branches, forks, commits, merges?
- Push, pull, fetch, stash, or rebase?

**→ Get in touch!**



**FHI GitLab**  
<https://gitlab.fhi.mpg.de>  
*(register first)*



**HIGH PERFORMANCE COMPUTING (HPC) AT FHI**

**RUNNING LARGE ANALYSES  
&  
COMPLEMENTING EXPERIMENTS WITH SIMULATIONS**



# HIGH PERFORMANCE COMPUTING (HPC) AT FHI

## Computing / Simulations

### Q-cluster

“Mini-”Supercomputer  
@ PP&B

### New cluster

@ MPCDF

## Analysis & Visualization

### JupyterHub

Interactive Python Server  
@ PP&B

### JupyterHub

Large Memory  
+ Many CPUs  
PPB + MPCDF

### Analysis Server ?

Graphical analyses  
→ Virtual server(s)  
PPB + MPCDF

NOW

SOON

END

2024

# HIGH PERFORMANCE COMPUTING (HPC) AT FHI

## Simulations

### Density Functional Theory

- Energetics
- Thermodynamics & Kinetics
- Structure, Geometry, Stability
- STM image simulation
- Vibrational Spectra
- Electron spectroscopy ...

### Kinetic Modeling

- Micro Kinetic Modeling
- Kinetic Monte Carlo ...

## Large Analyses

Resource intensive scripts and programs

## AI Training

Anything that requires more than a desktop PC



<https://doku.lrz.de/supermuc-ng-10745965.html>



# HIGH PERFORMANCE COMPUTING (HPC) AT FHI

## Simulations

### Density Functional Theory

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- STM image simulation
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## Large Analyses

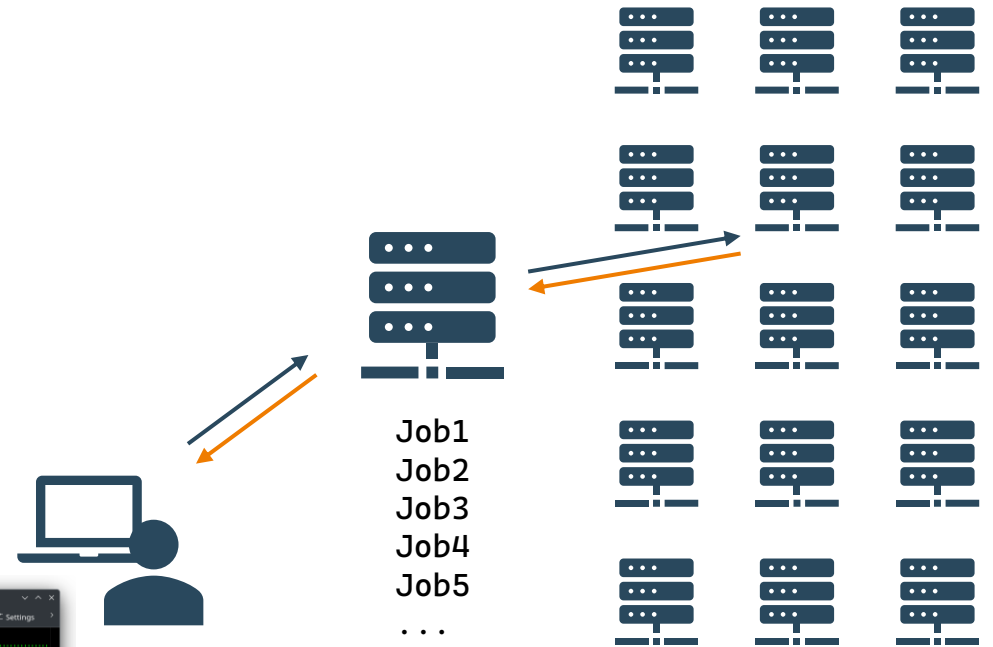
Resource intensive scripts and programs

## AI Training

Anything that requires more than a desktop PC



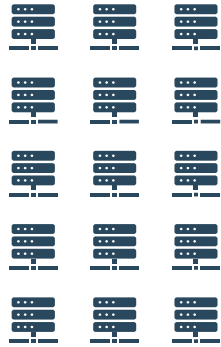
<https://doku.lrz.de/supermuc-ng-10745965.html>



*Job = script to execute*



# HIGH PERFORMANCE COMPUTING (HPC) AT FHI



**TH** →

**Raven (MPCDF)**

- 1592 nodes (server)
- 114624 cores
- 447 TB RAM

**Department based access**  
*(and single users)*

**Q-Cluster (PP&B)**

- 40 nodes (server)
- 1280 cores
- 7.7 TB RAM

ISC →

AC →

PC →

MP →

**Unrestricted FHI access**

**Supermuc (LRZ)**

- 6480 nodes (server)
- 311040 cores
- 719 TB RAM

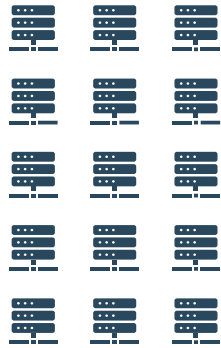
**Juwels (JSC)**

- >2600 nodes (server)
- >130000 cores

**Grant based access**



# HIGH PERFORMANCE COMPUTING (HPC) AT FHI



- Medium-sized simulations & analyses
- Simulations independent from theory groups

## Q-Cluster (PP&B)

- 40 nodes (server)
- 1280 cores
- 7.7 TB RAM

**Unrestricted FHI access**

ISC

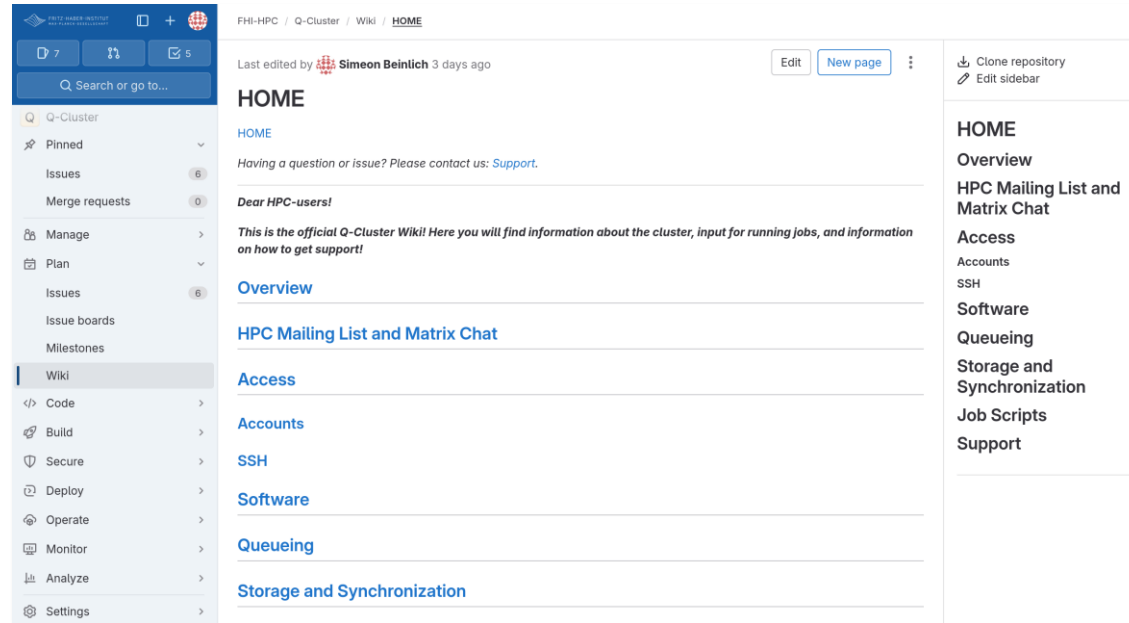
AC

PC

MP



# HIGH PERFORMANCE COMPUTING (HPC) AT FHI



- Medium-sized simulations & analyses
- Simulations independent from theory groups

## Q-cluster wiki

<https://gitlab.fhi.mpg.de/fhi-hpc/q-cluster/~wikis>  
(register first)

PPB Wiki > HPC

Mailing List

Q-cluster wiki

Matrix Channel

Technical Issues?

Plan to run simulations?

Compiling new code?

Get in touch!

Ideas?

Advice?

Support?

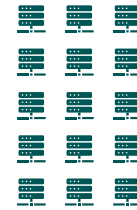




# HIGH PERFORMANCE COMPUTING (HPC) AT FHI

## Q-Cluster (PP&B)

- System & software updates
- Hardware repairs



## *New Cluster*

- Currently in planning
- **Hosted at MPCDF**

**Hardware and Software  
reaching their End of Life**

- + **Less maintenance and administration work**  
→ More support
- + **State-of-the-art configuration**  
Software & Hardware
- + **Ideally: Software stack identical to Raven**  
Compatibility and Transferability

|                 |                         |                         |
|-----------------|-------------------------|-------------------------|
| Sun Grid Engine | <b>Scheduler</b>        | SLURM                   |
| CentOS (Linux)  | <b>Operating System</b> | SUSE Enterprise (Linux) |
| RocksCluster    | <b>Cluster Setup</b>    | -                       |



# INTERACTIVE PYTHON SERVER - JUPYTERHUB

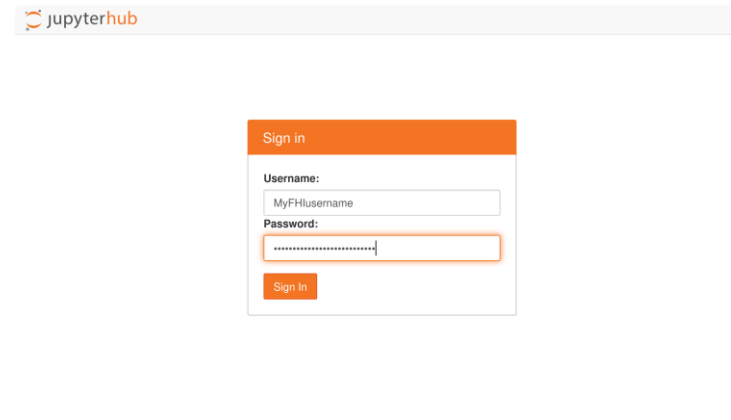
## Jupyter Notebook = *Interactive Script*

### Combining the best of

- Python scripts
- Python terminal
- Markdown documentation

### JupyterHub:

- Requires no local installation
- **Directly use ready-made notebooks!**
- **Soon: very powerful hardware!**

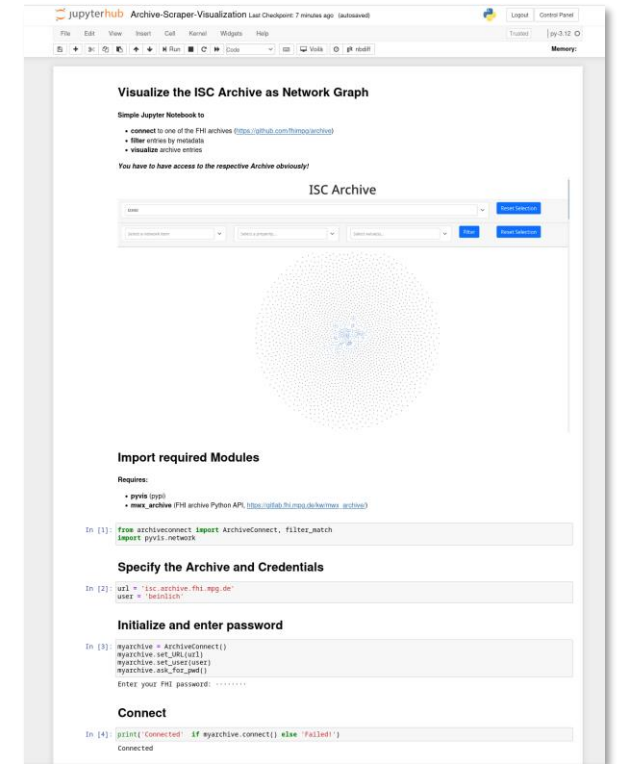


**Tiny Little JupyterHub**  
tljh.fhi.mpg.de

Simple

No installation

Uniform Setup





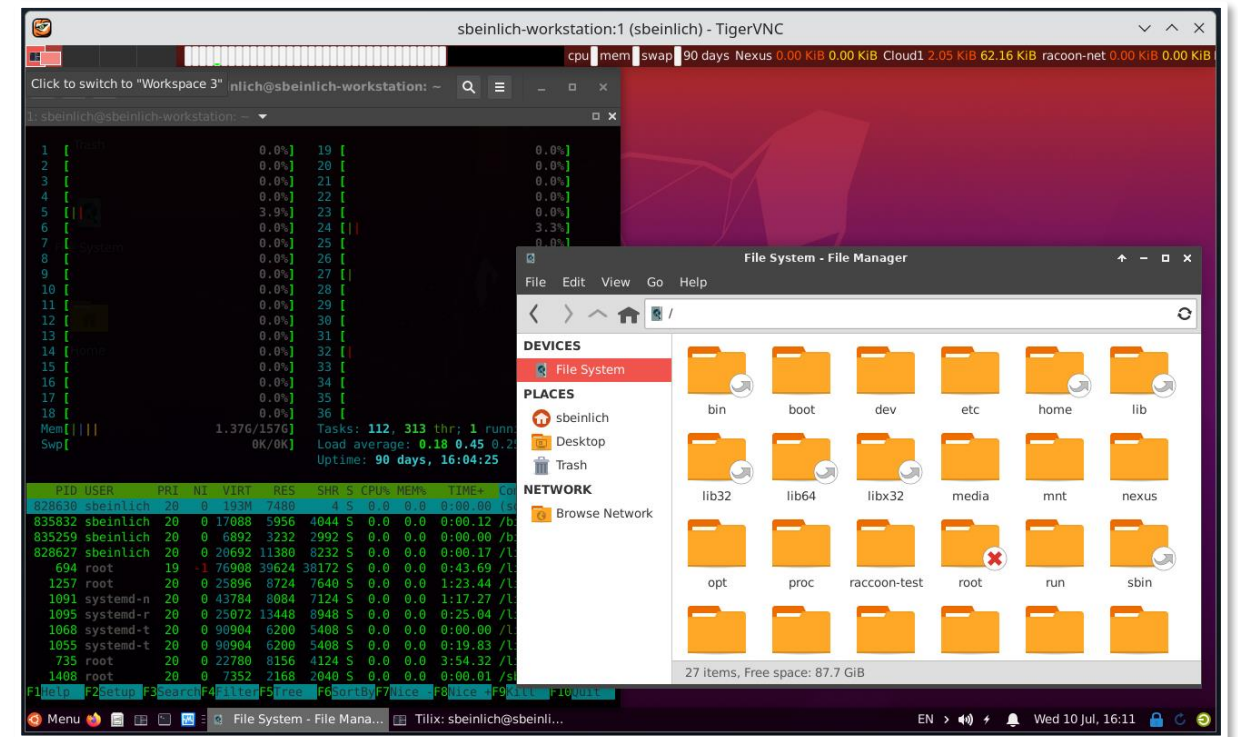
# GRAPHICAL ANALYSES – VIRTUAL SERVER(S)

Not Python and not runnable on a Cluster?

→ Graphical Virtual Analysis Server!

- Graphical Desktop sessions (VNC)
- High resource (Memory, CPU, ...)
- Direct support
- Ready to use scripts etc. possible.
- Own Software installable on request.

→ ~ Theory department workstations





# SUMMARY

## Challenges and Pathways in Scientific IT

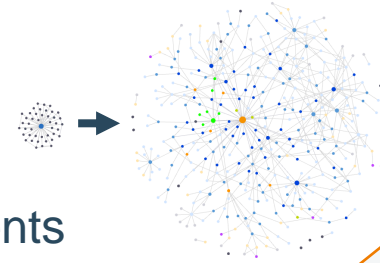
- More (complex) data & setups + More requirements  
→ Suitable Infrastructure and Automation
- **From Repetitive & Local to Automatized & Connected**
- Joint approach to tackle challenges
- **From manual to scripted analyses (where possible)**

## Role of PP&B

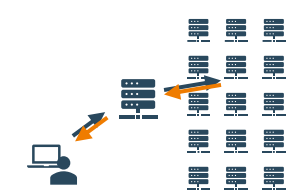
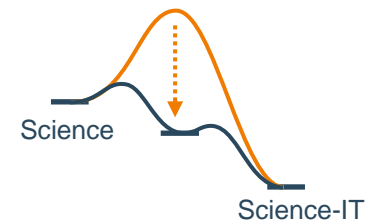
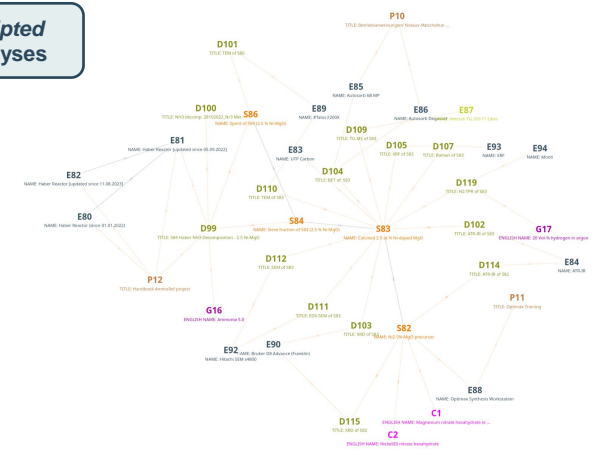
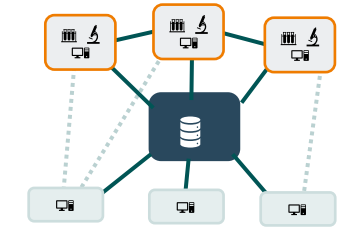
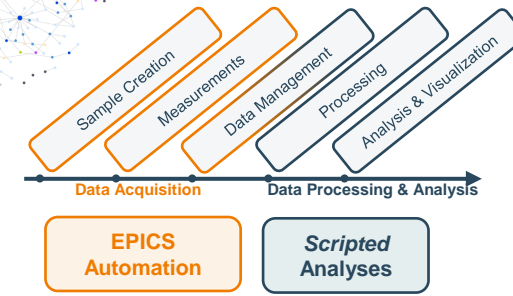
- Focus on Science IT
- More support and scientific services

## HPC at FHI

- New infrastructure, more support
- Less maintenance and administration



# THANK YOU!



*Need something similar? Get in touch!*



# PC DEPARTMENT – TOPICS, QUESTIONS, IDEAS 1/2

## STORAGE?

Microscopy raw data?

- ~10TB / a
- ✓ Both locally and remote (MPCDF) directly feasible.

## Raw-Data-Processing?

- > 10h processing time, Parallelization?
- ✓ Real or trivial Parallelization on cluster or Analysis Server (Software-dependent?!)

## Automation!

LabView preferred: fast and simple set up.

- Some PP&B Ideas:
  - Archive integration + Scripted Analyses?
  - LabView-EPICS Interface (Server/Client)?

## Data-Analysis?

SVD / ICA?

(Single Value Decomp. / Indep. Comp. Analysis)

- > 100 000 entry Arrays
- ✓ Where? → Cluster / Jupyterhub / Analysis server
- ✓ Support? → Me!
- ✓ Data Format? → Any common/ open/ readable/ non-proprietary (.csv, .pkl, .txt, .hdf5, ...)
- ✓ Software? → Python / Scikit-Learn?
- ✓ Waiting Time?
  - Analysis Server (new): → 0
  - JupyterHub (new): → 0
  - Cluster (old/new): → ~1 - 4h.
- ✓ MPCDF - Raven/Viper? → TH Budget?



# PC DEPARTMENT – TOPICS, QUESTIONS, IDEAS 2/2

## EPICS AUTOMATION?

Large activation barrier!

- ✓ Introductory Courses? → Yes, please get in touch!
- Maybe: Joint Demo Project?
- ✓ Fully set-up systems from PP&B
- ✓ General:
  - What is EPICS?
  - How large is the activation barrier?
  - What is an IOC?
  - Platform dependence?
  - Drivers for Instruments?
  - Large Data Rates - (Microscopy-) pictures?

## COMSOL?

HPC – runnable?

- Cluster: → Yes, if job is scriptable  
Does a CLI exist for your application type?
- Analysis Server → Yes  
(GUI + full software & network control)

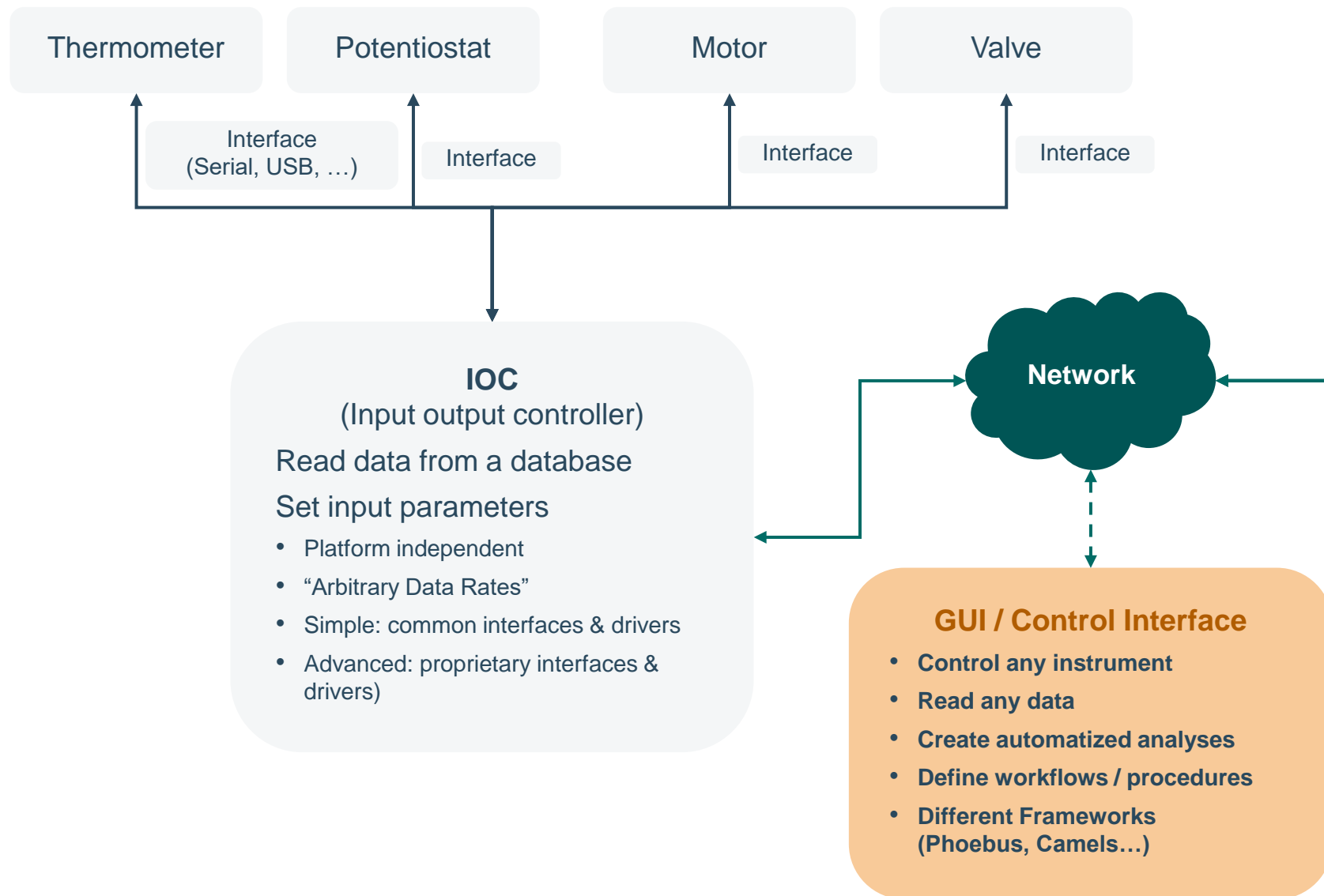
## Licensing?

Floating Network Licenses @ HPC, e.g. Comsol?

- Q-cluster: → yes (same network)
- New cluster / Analysis Server:  
→ soon (network integration is currently implemented)



# APPENDIX – EPICS IN A (TINY) NUTSHELL



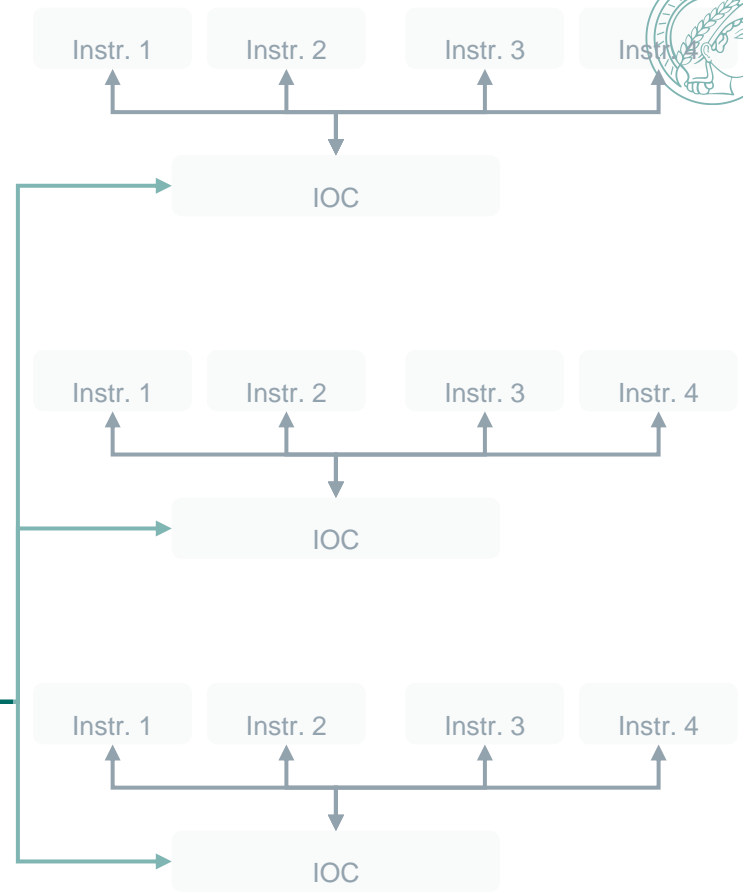
**IOC**  
(Input output controller)

Read data from a database  
Set input parameters

- Platform independent
- “Arbitrary Data Rates”
- Simple: common interfaces & drivers
- Advanced: proprietary interfaces & drivers)

**GUI / Control Interface**

- Control any instrument
- Read any data
- Create automatized analyses
- Define workflows / procedures
- Different Frameworks (Phoebus, Camels...)



**NOMAD CAMELS**  
Control instruments,  
run measurement  
protocols, and record  
**FAIR data!**