



PP&B – Computer Support Group

FRITZ-HABER-INSTITUT
MAX-PLANCK-GESELLSCHAFT

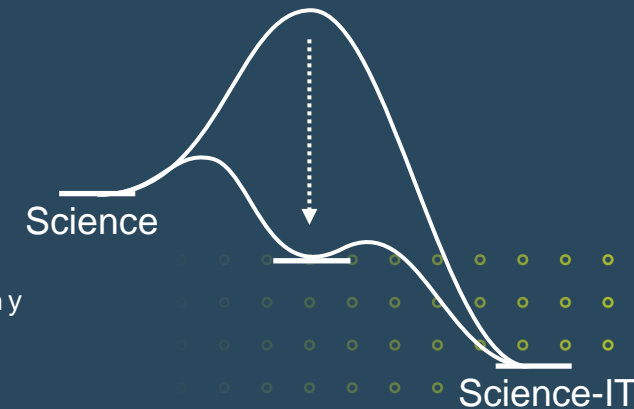


IT – FROM THE CURSE TO A BLESSING? TACKLING CURRENT AND FUTURE CHALLENGES OF SCIENTIFIC IT

Simeon D. Beinlich^{1,*} and Heinz Junke¹

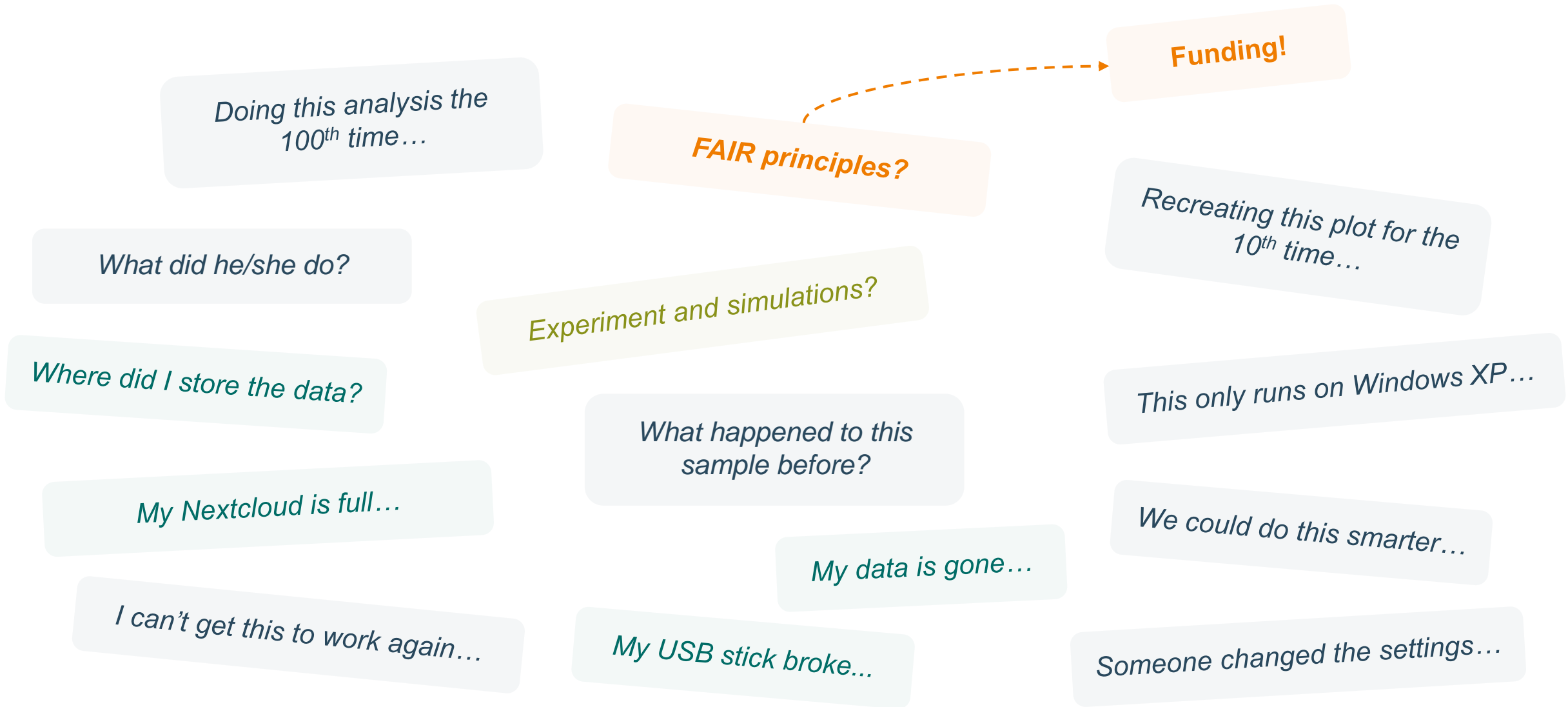
¹ PP&B – Computer Support Group
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

*beinlich@fhi.mpg.de





(SOME) CHALLENGES IN SCIENTIFIC IT

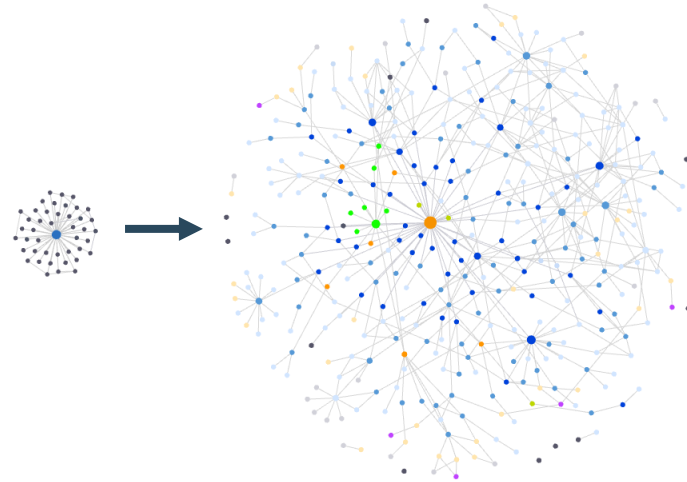




CHALLENGES IN SCIENTIFIC IT

More data

More complex data



More complex analyses

More complex setups

More requirements



CHALLENGES IN SCIENTIFIC IT

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More complex data

... More IT ...

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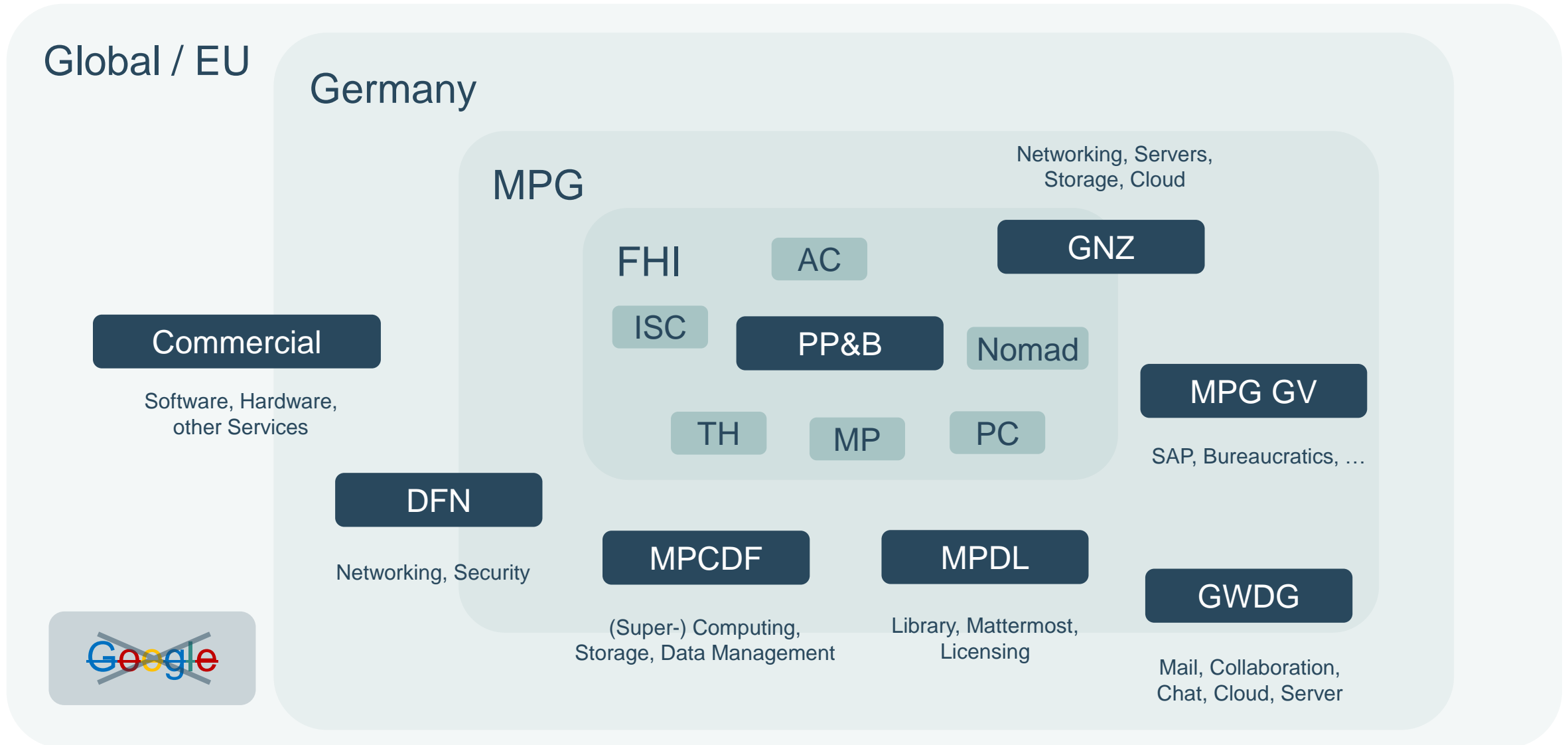
IT INFRASTRUCTURE AT MPG & FHI

&

THE ROLE OF PP&B

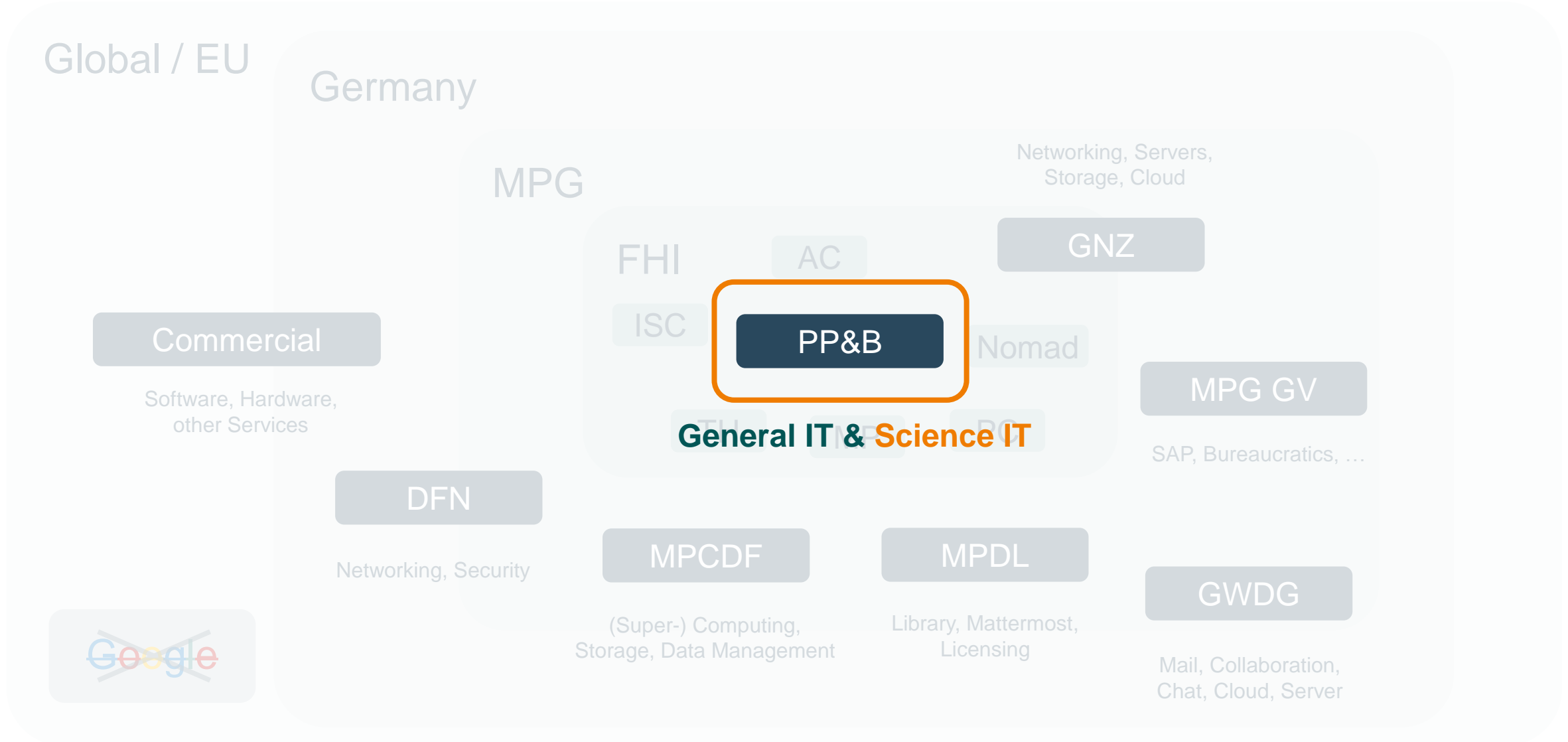


IT INFRASTRUCTURE AT MPG & FHI



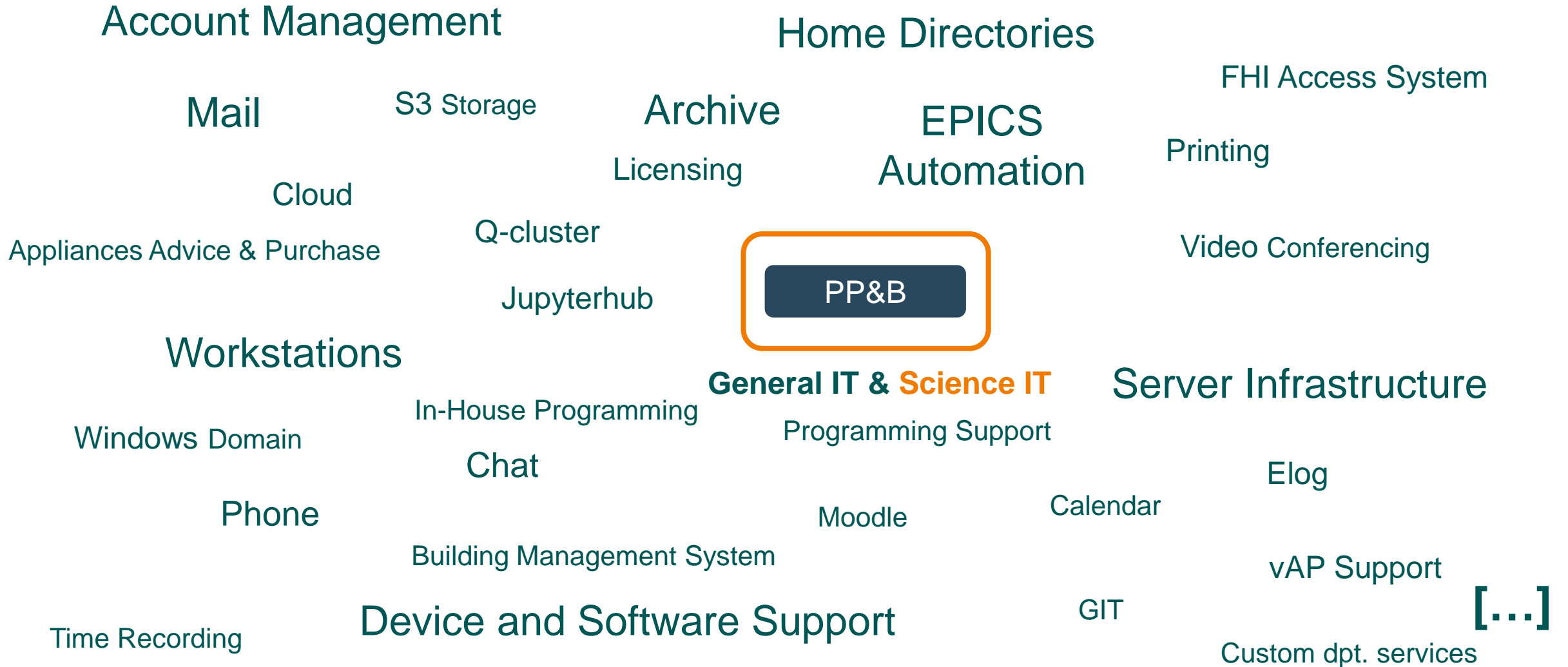


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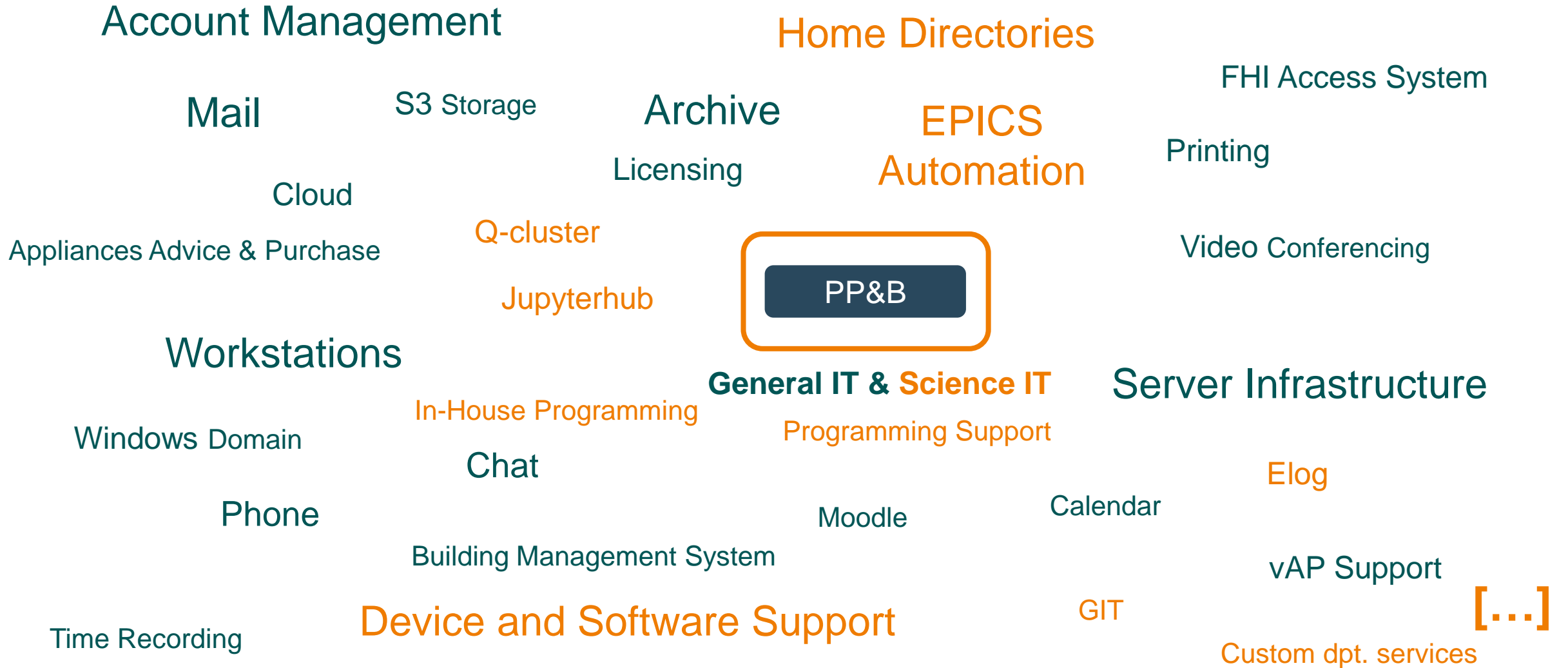


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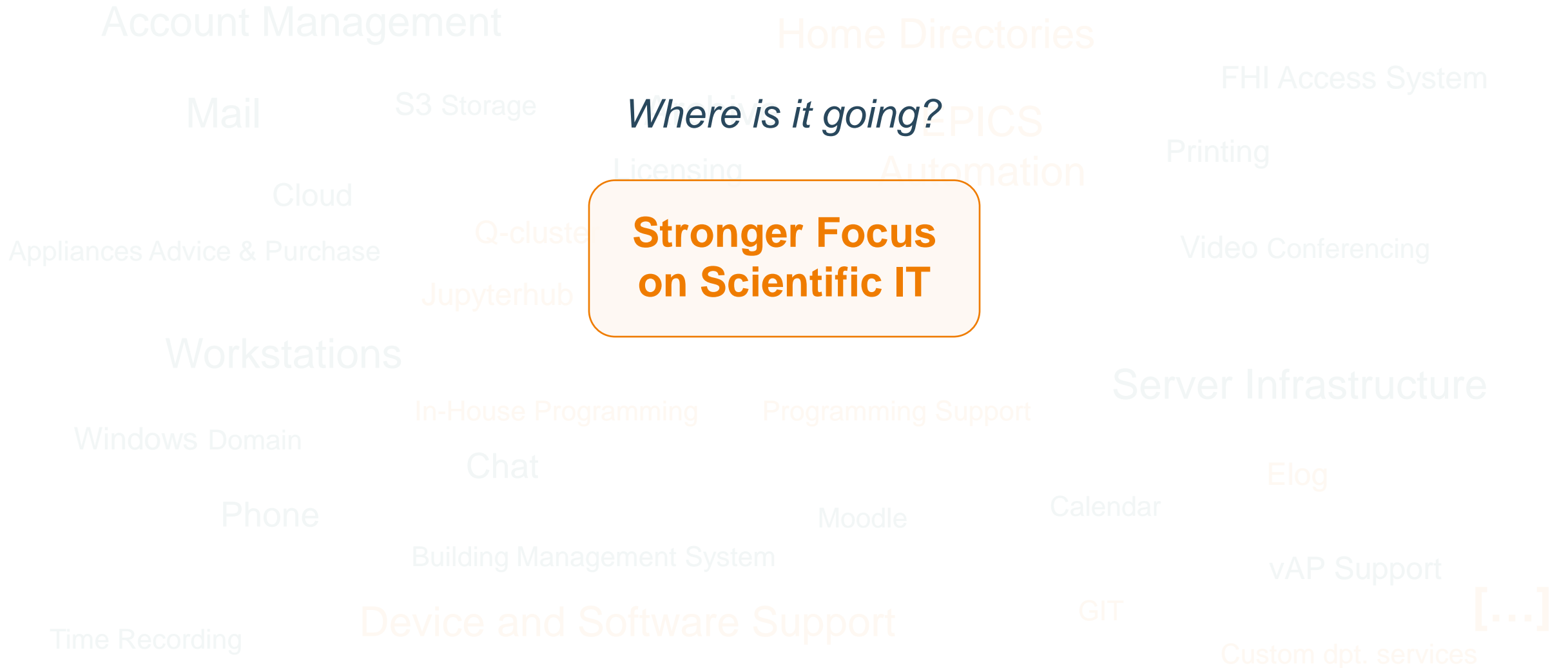


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PP&B – COMPUTER SUPPORT GROUP





PP&B – COMPUTER SUPPORT GROUP

Account Management

Home Directories

FHI Access System

Mail

S3 Storage

Archive

EPICS

Printing

Licensing

Automation

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*
→ **GW DG**
- *E.g. Cluster Hardware, JupyterHub, Storage, Virtual Servers*
→ **MPCDF**



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Automation

Automation Support

In-house programming

Move Services

(In-house)

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→ **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 ...



Katharina Merle

Apprentice
*Mathematical technical software development
... soon (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

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& Documentation**

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**INFRASTRUCTURE
AUTOMATION
COLLABORATION**

**Setup Complexity
& Stability**

**Accessibility &
Findability**

Internally & externally

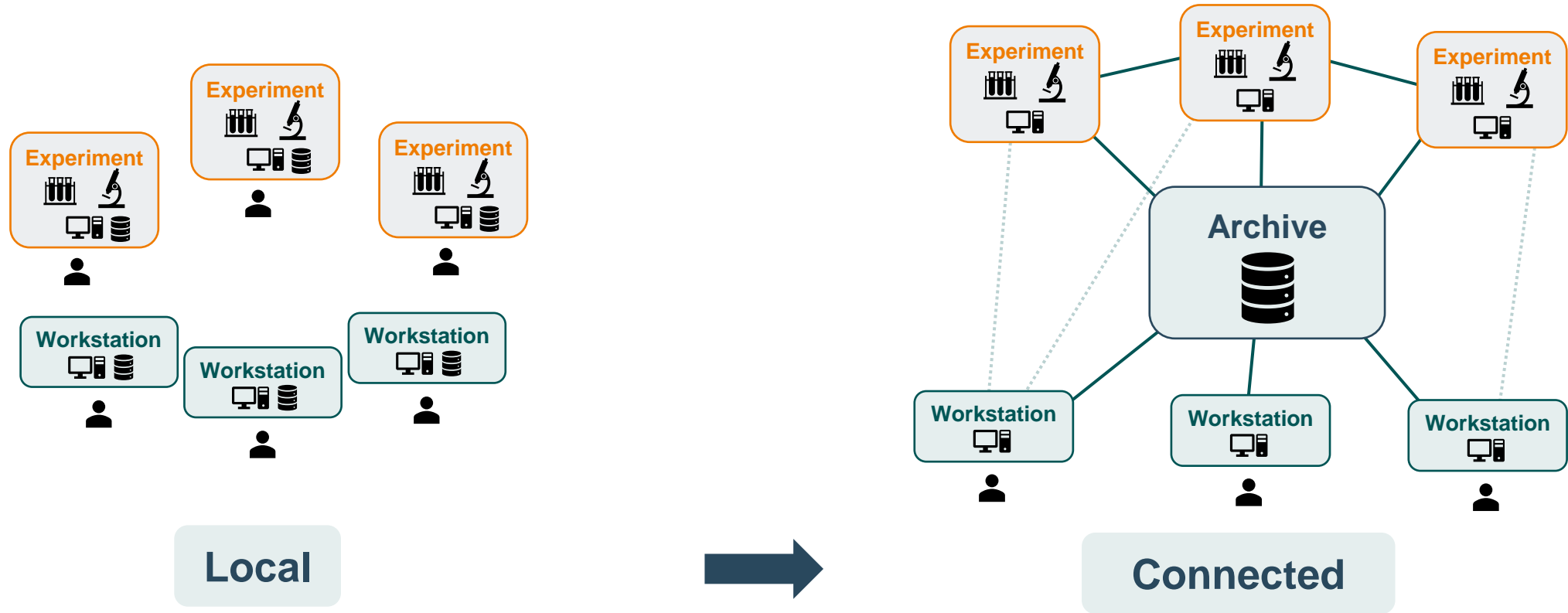
Reusability & Uniformity
Data & procedures!

**Independence from
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AI?!



INFRASTRUCTURE, AUTOMATION, & COLLABORATION



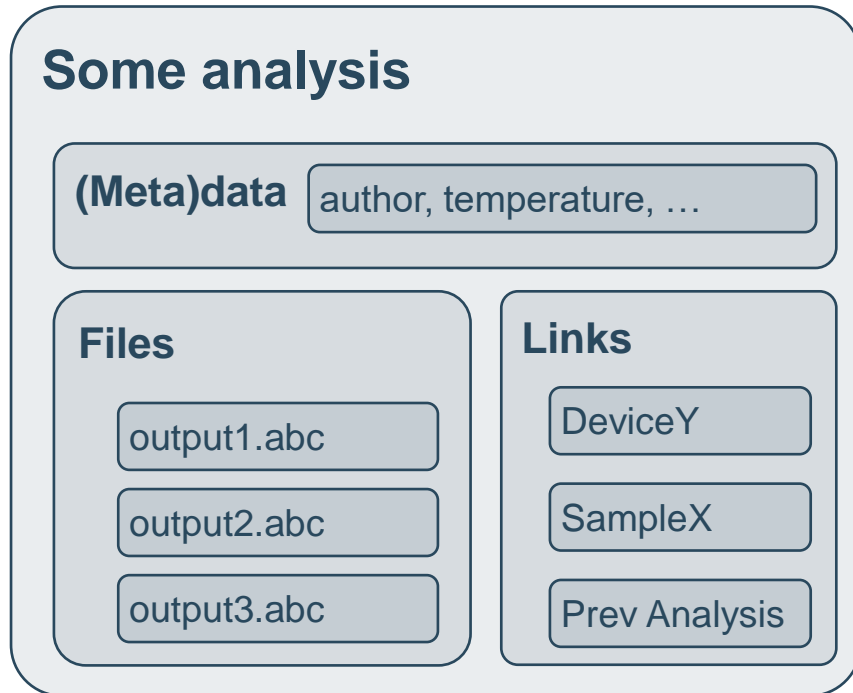
Local
Single Person
Repetitive manual workflow

Connected
Group
Streamlined automatized workflow

GOALS	• Findable data	• Reproducible data	• Streamlined & reusable procedures
	• Uniform data	• Documented data	
	• Secure data	• Data provenance	

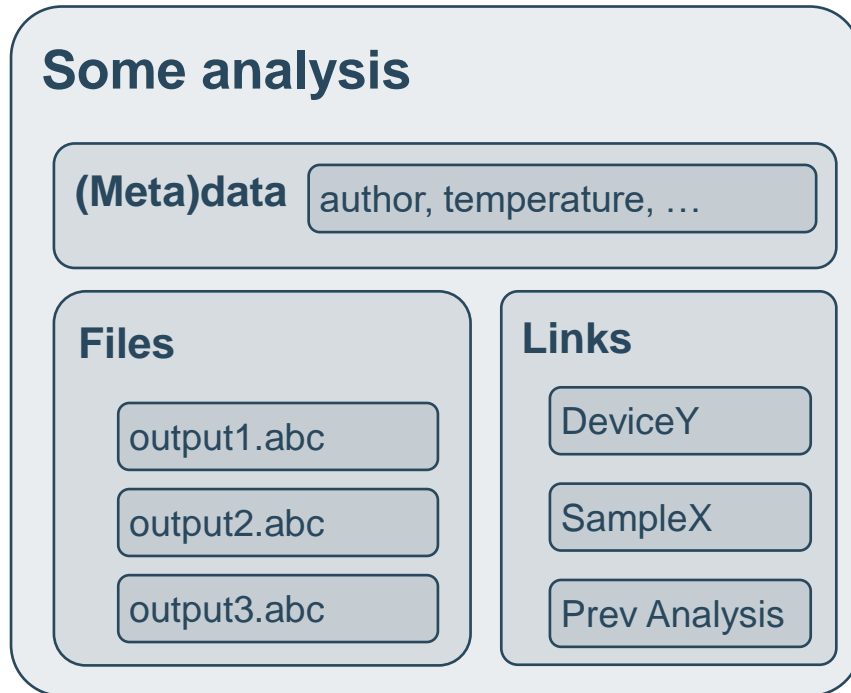


INFRASTRUCTURE – THE FHI ARCHIVE





INFRASTRUCTURE – THE FHI ARCHIVE



Data Management

Data Security

Accessibility & Findability

Reusability & Uniformity

Reproducibility & Documentation

Data Provenance

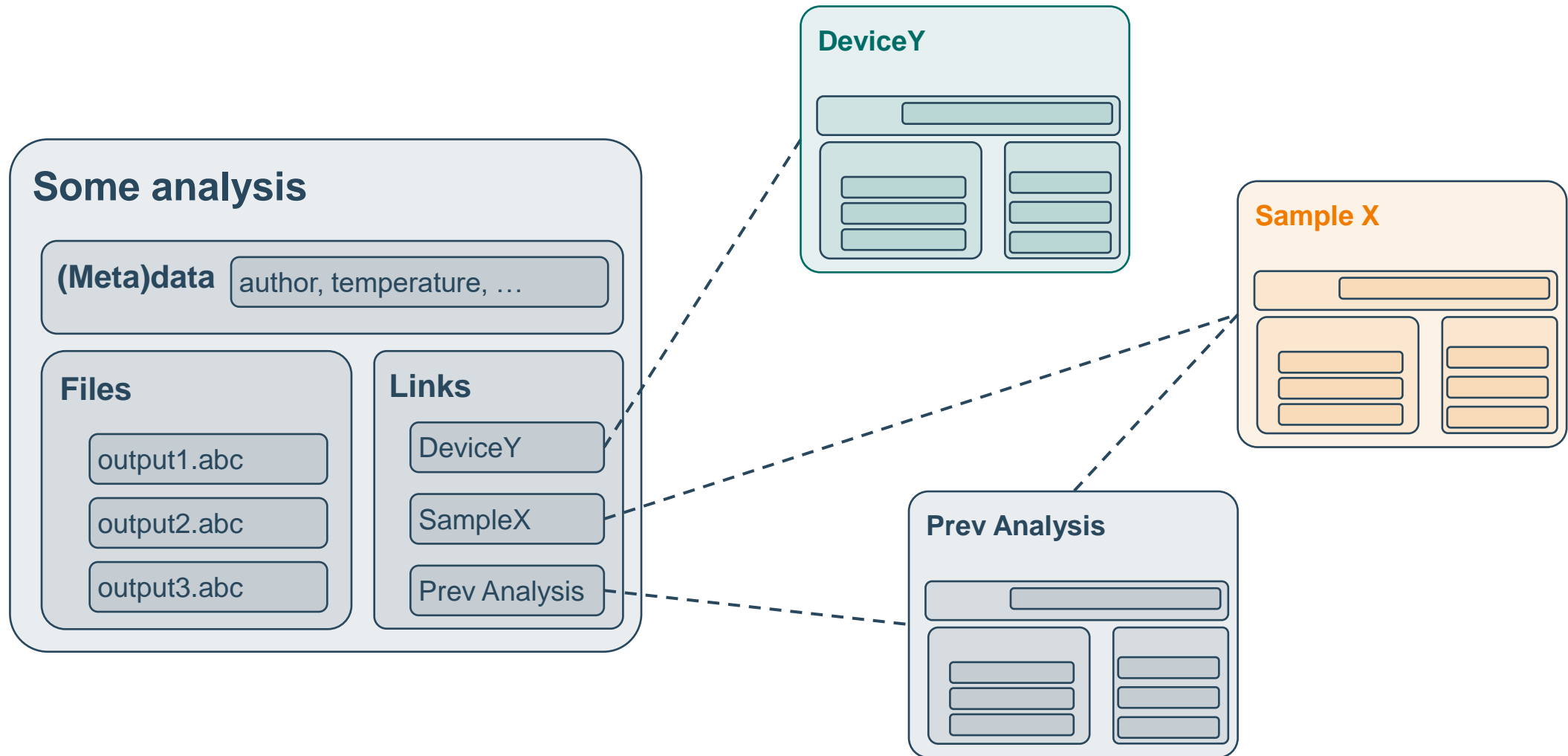
Setup Complexity & Stability

Independence from vendors

AI?!

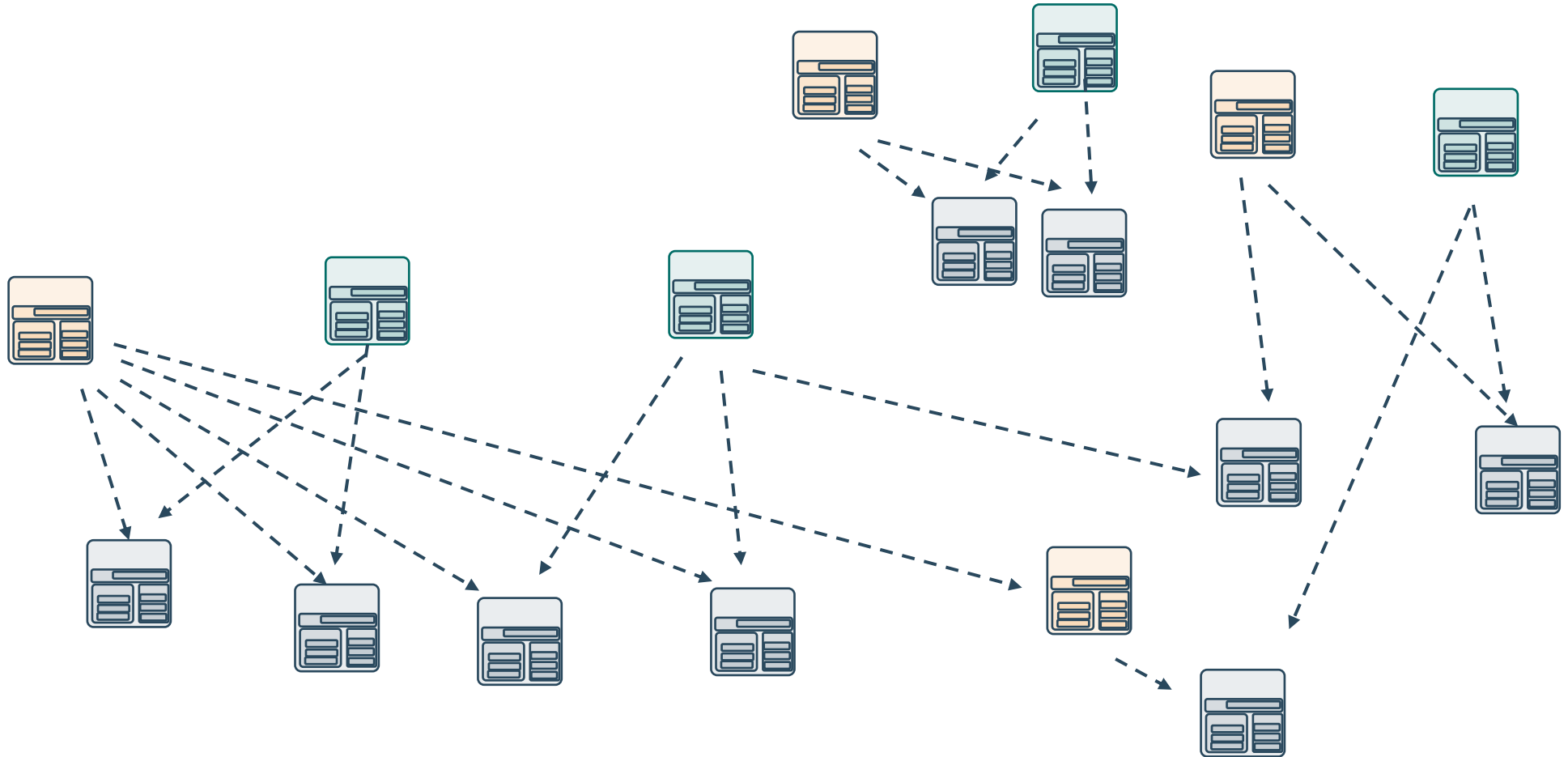


INFRASTRUCTURE – THE FHI ARCHIVE





INFRASTRUCTURE – THE FHI ARCHIVE

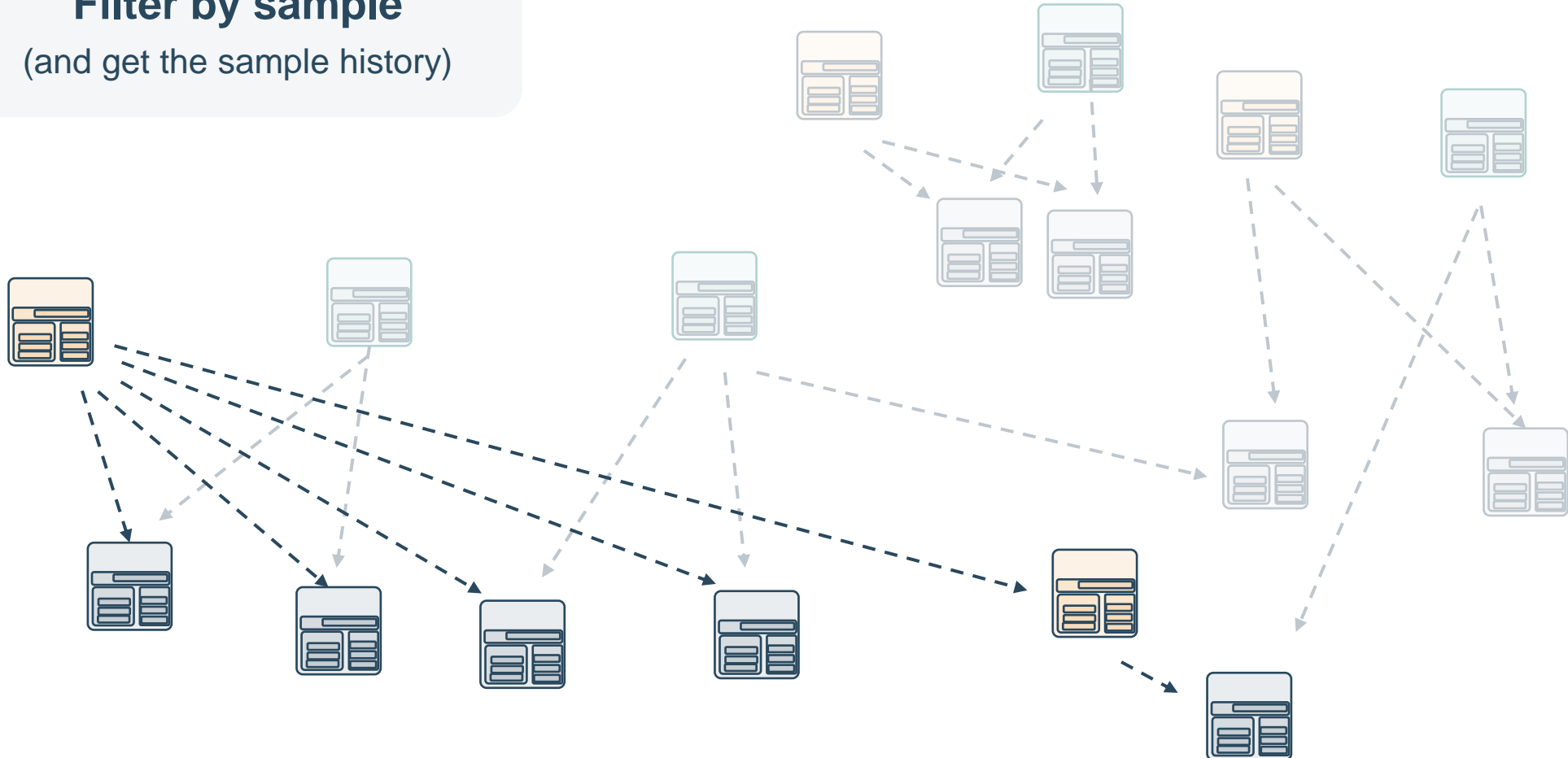




INFRASTRUCTURE – THE FHI ARCHIVE



Filter by sample
(and get the sample history)

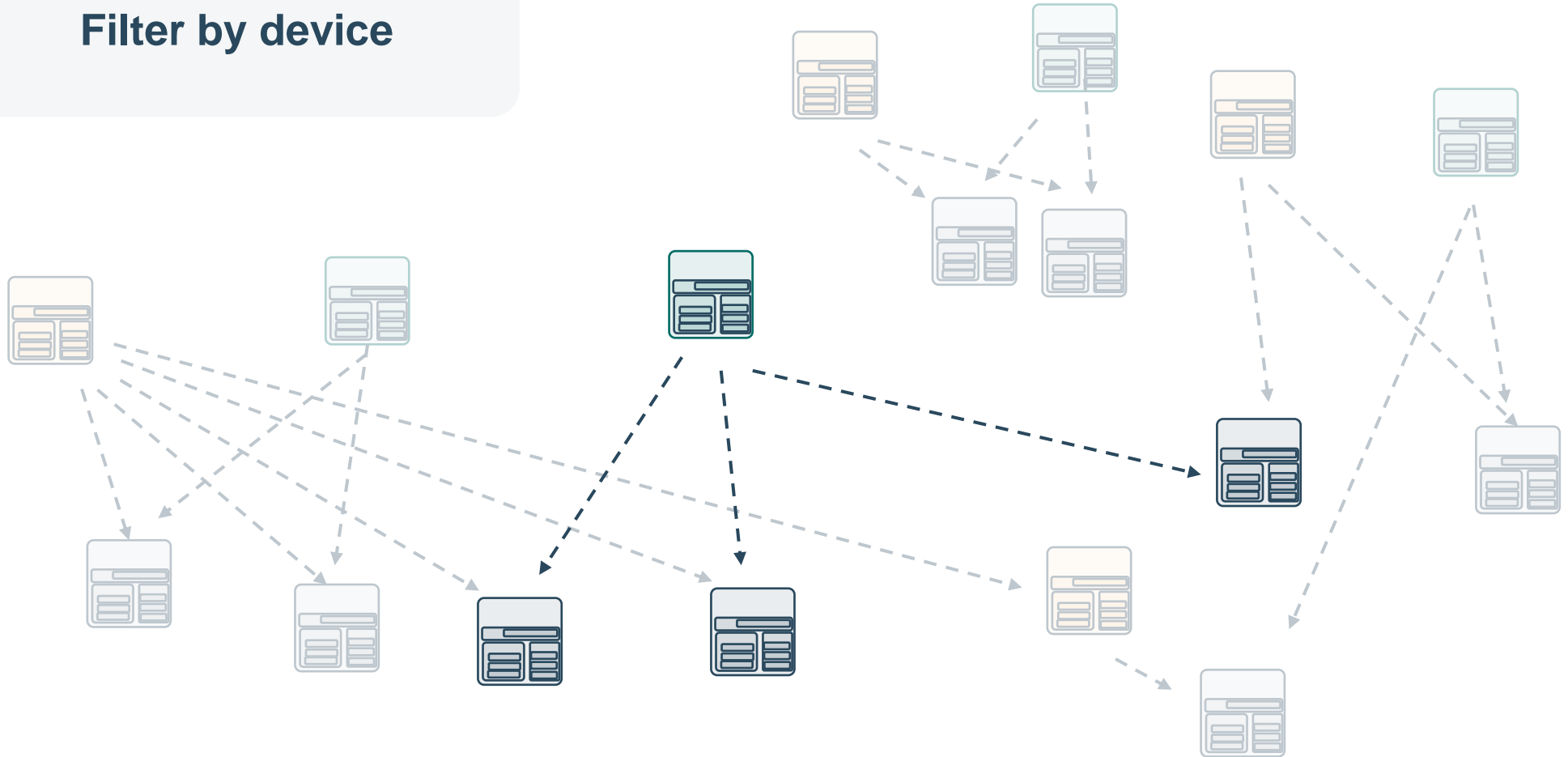




INFRASTRUCTURE – THE FHI ARCHIVE



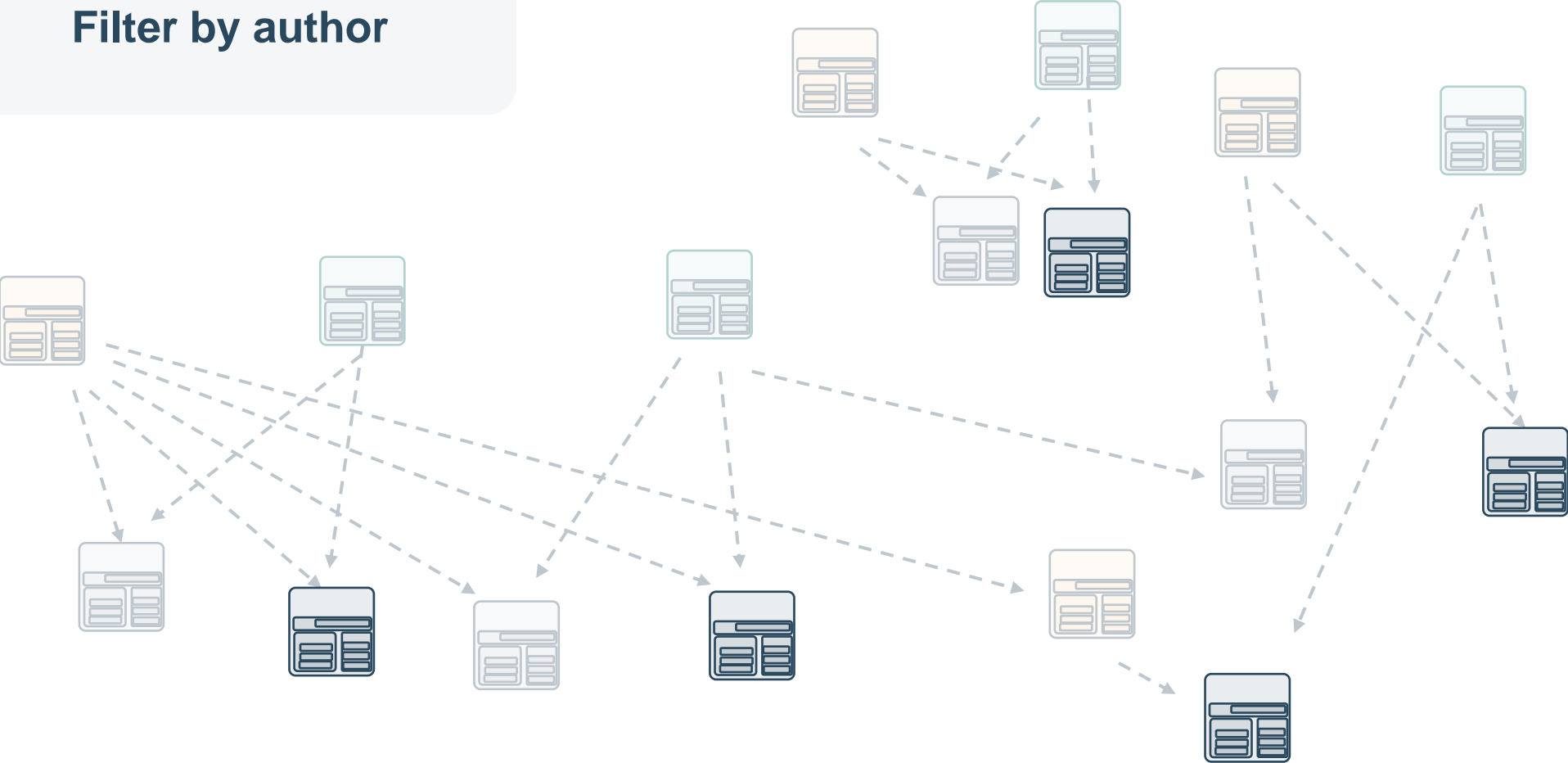
Filter by device





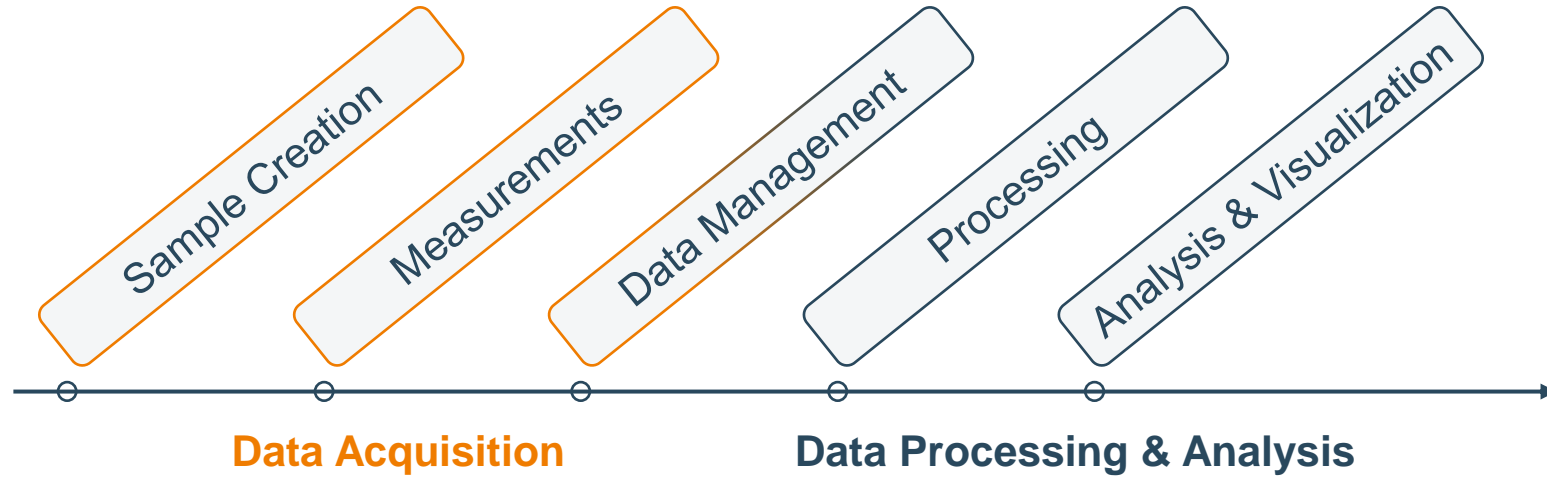
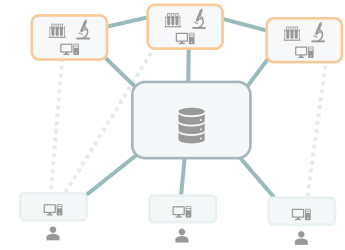
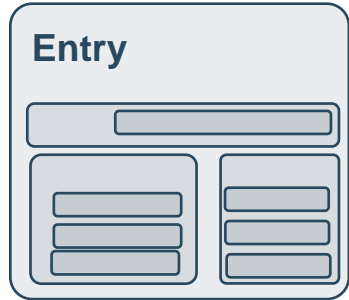
INFRASTRUCTURE – THE FHI ARCHIVE

Filter by author





CHALLENGES IN SCIENTIFIC IT

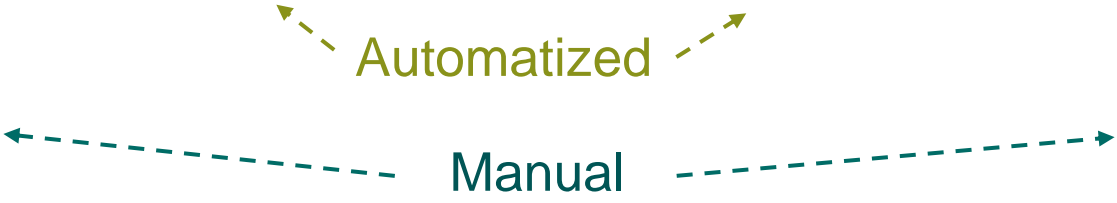


EPICS Automation

Scripted Analyses
(Python, Archive API, Flask?)

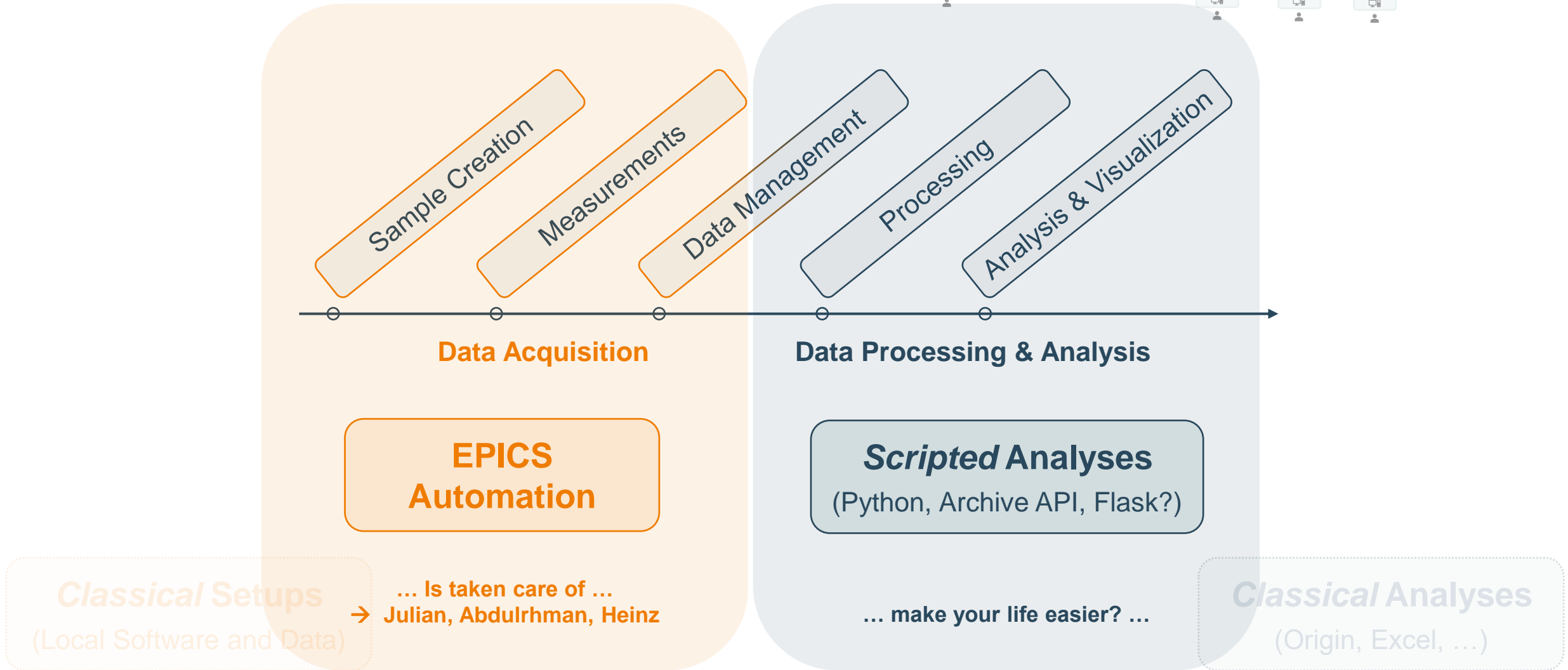
Classical Setups
(Local Software and Data)

Classical Analyses
(Origin, Excel, ...)





CHALLENGES IN SCIENTIFIC IT





SCRIPTED ANALYSES – E.G. PYTHON

Automatize repetitive tasks

- Data collection
- Data processing
- Analysis
- Plotting

Python: *simple & powerful*

- Use local workstation...
- ...or JupyterHub

Good to know

- Archive Python API!
[mwx_archive @ gitlab.fhi.mpg.de!](https://gitlab.fhi.mpg.de/mwx_archive)



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[@gitlab.fhi.mpg.de!](https://gitlab.fhi.mpg.de/mwx_archive)

But I don't know Programing?

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

Examples

- Interactive ISC Archive Visualization
Notebook on JupyterHub
- Filter WebApp
Module on local Python



SCRIPTED ANALYSES – PYTHON JUPYTER NOTEBOOKS

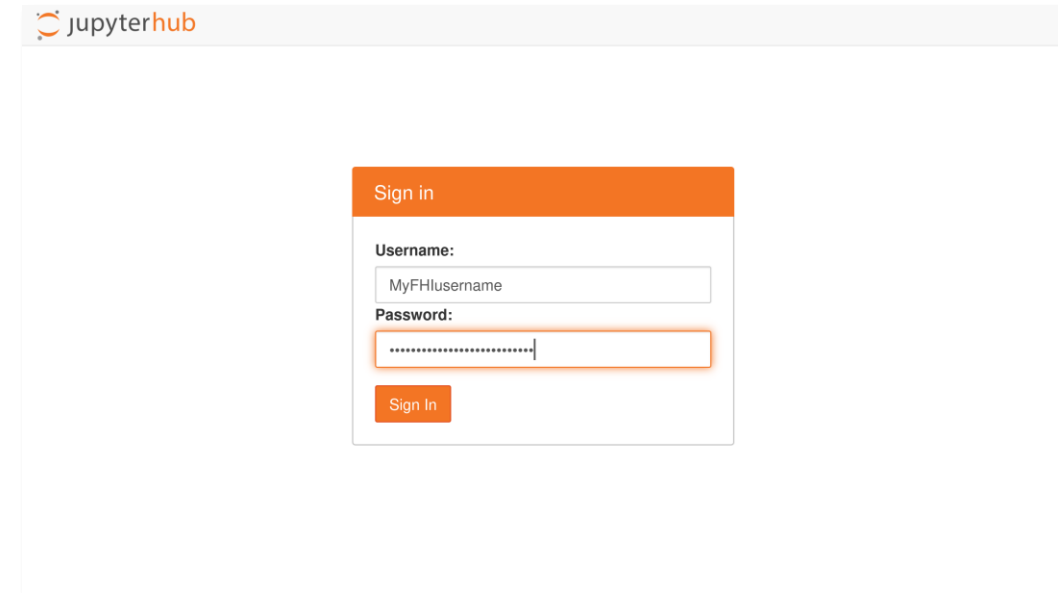
Jupyter Notebook = *Interactive Script*

Combining the best of

- Python scripts
- Python terminal
- Markdown documentation

JupyterHub:

- Requires no local installation
- **Directly use ready-made notebooks!**



Tiny Little JupyterHub
<https://tljh.fhi.mpg.de>

Simple

No installation

Uniform Setup



EXAMPLE 1: INTERACTIVE ARCHIVE VISUALIZATION

What it does

- Visualize how entries in the archive are connected
- **Overview and Searching**

Steps it does for you

- **Connect** to the archive
- Get all **metadata**
- **Filter** archive entries
- Get **connections** between entries
- **Visualize** as network graph

The screenshot shows a Jupyter Notebook interface with the following content:

Visualize the ISC Archive as Network Graph

Simple Jupyter Notebook to

- connect to one of the FHI archives (<https://github.com/fhmpg/archive>)
- filter entries by metadata
- visualize archive entries

You have to have access to the respective Archive obviously!

ISC Archive

Search interface with dropdowns for 'date', 'select a network type', 'select a company', and 'select network', along with 'filter' and 'select selection' buttons.

Import required Modules

Requires:

- `pyvis` (pypi)
- `mxr_archive` (FHI archive Python API, https://gitlab.fhi.mpg.de/kw/mxr_archive/)

```
In [1]: from archiveconnect import ArchiveConnect, filter_match
import pyvis.network
```

Specify the Archive and Credentials

```
In [2]: url = 'isc.archive.fhi.mpg.de'
user = 'beinlich'
```

Initialize and enter password

```
In [3]: myarchive = ArchiveConnect()
myarchive.set_URL(url)
myarchive.set_user(user)
myarchive.ask_for_pwd()
Enter your FHI password: .....
```

Connect

```
In [4]: print('Connected' if myarchive.connect() else 'Failed')
Connected
```

<https://gitlab.fhi.mpg.de/beinlich/archive-visualization-notebook> (register first)

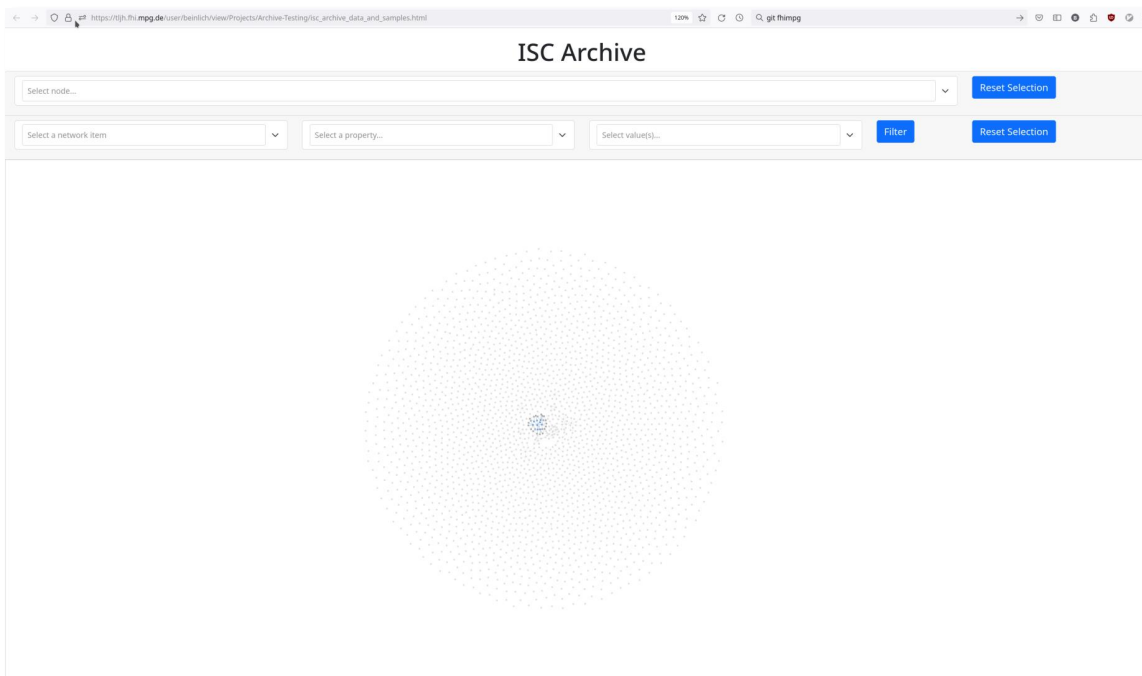
Interested in using it? Get in touch!



EXAMPLE 1: INTERACTIVE ARCHIVE VISUALIZATION

What it does

- Visualize how entries in the archive are connected
- **Overview and Searching**



```
Simple Jupyter Notebook to
• connect to one of the FHI archives (https://gitlab.com/frmpop/archiv)
• filter entries by metadata
• visualize archive entries

ISC Archive

Select node... [Reset Selection]
Select a network item | Select a property... | Select values... [Filter] [Reset Selection]

Import required Modules
Requires:
• pyvis (pyvis)
• max_archive (FHI archive Python API, https://gitlab.fhi.mpg.de/kw/mex_archive)

In [14]: from archiveconnect import ArchiveConnect, filter_match
import pyvis.network

Specify the Archive and Credentials
In [2]: url = 'isc.archive.fhi.mpg.de'
user = 'beinlich'

Initialize and enter password
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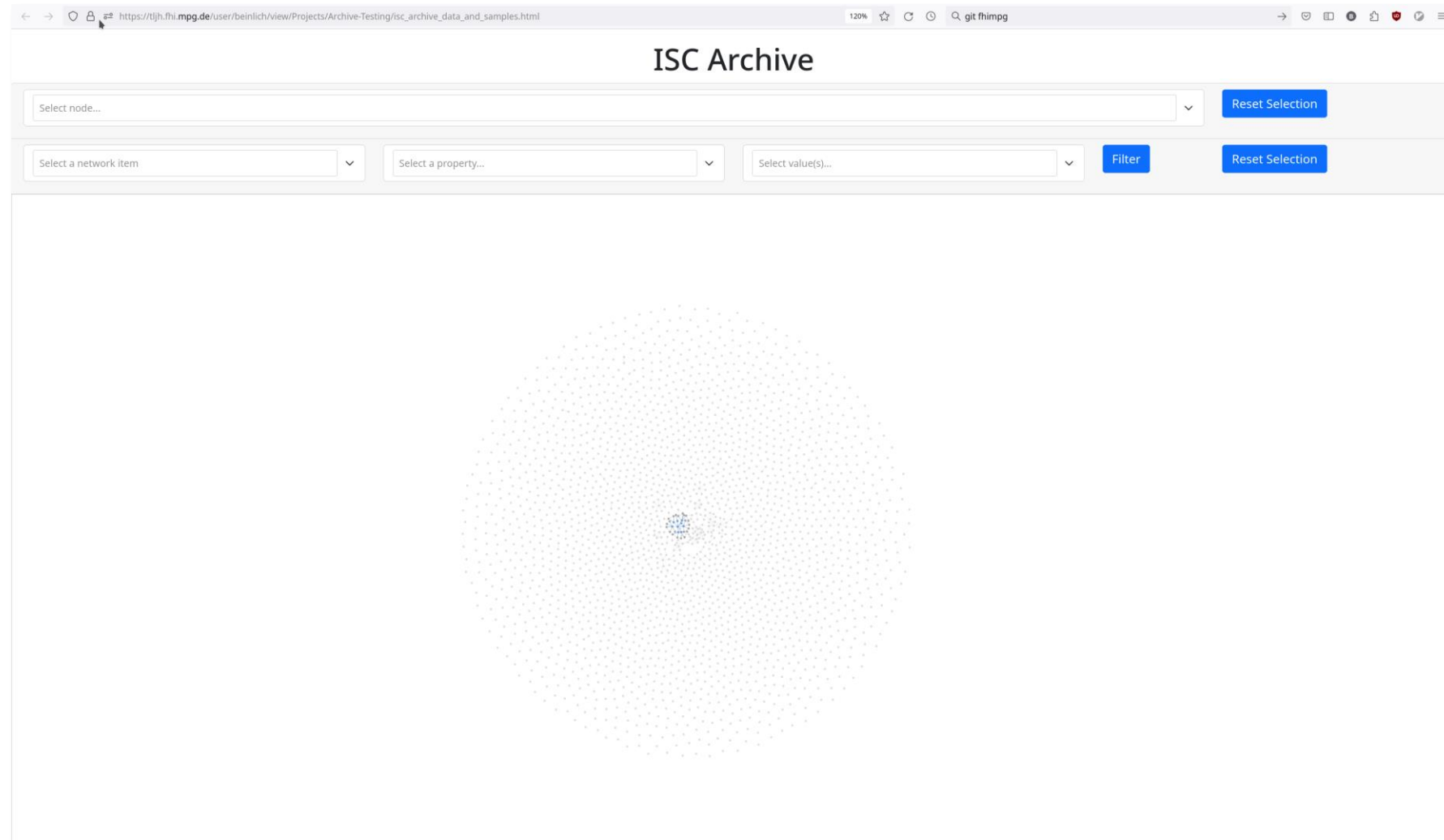
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<https://gitlab.fhi.mpg.de/beinlich/archive-visualization-notebook> (register first)

Interested in using it? Get in touch!



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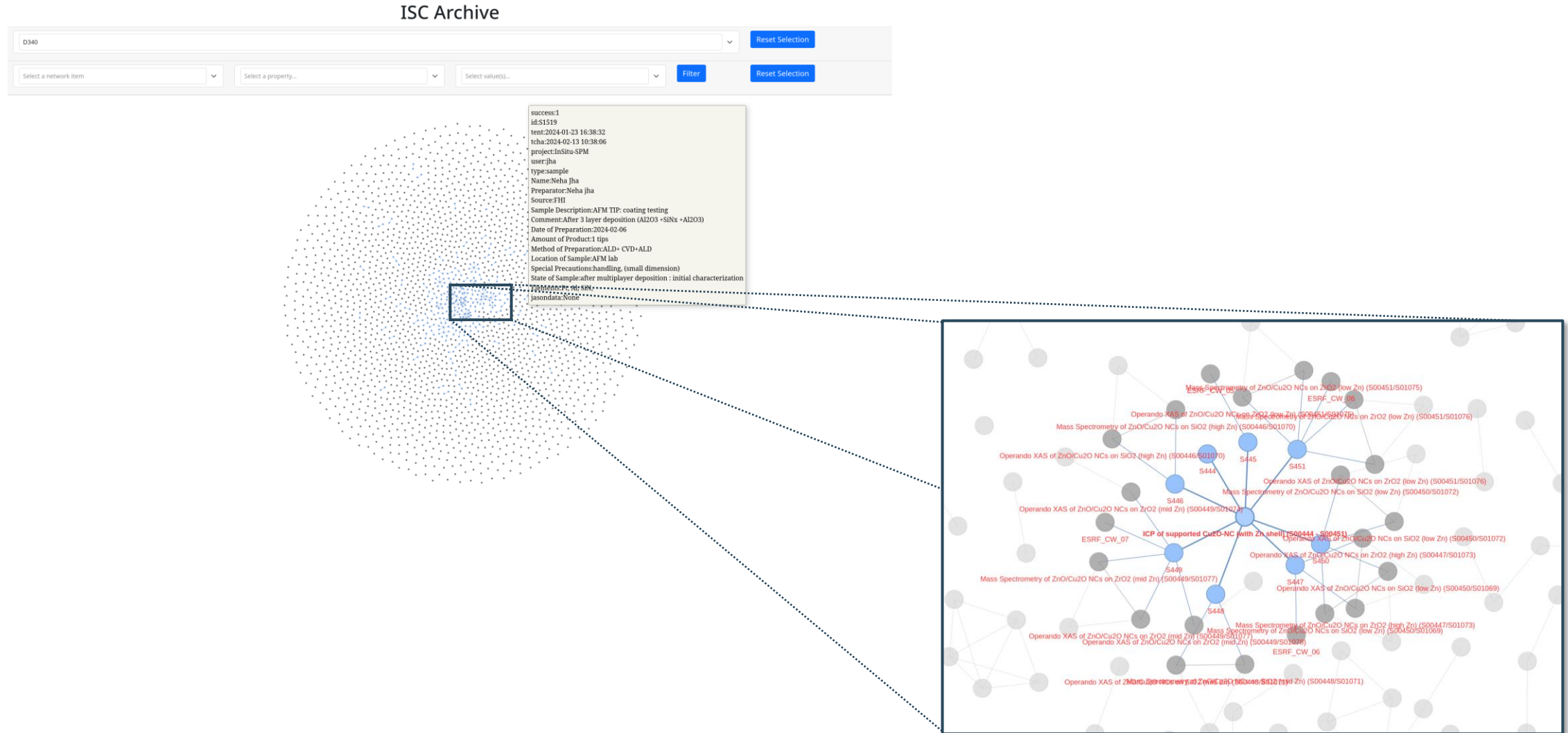


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EXAMPLE 1: INTERACTIVE ARCHIVE VISUALIZATION





EXAMPLE 1: INTERACTIVE ARCHIVE VISUALIZATION

ISC Archive

D340 Reset Selection

Select a network item Select a property... Select value(s)... Filter Reset Selection

```
success:1
id:S1519
tent:2024-01-23 16:38:32
tcha:2024-02-13 10:38:06
project:InSitu-SPM
user:jha
type:sample
Name:Neha Jha
Preparator:Neha Jha
Source:FHI
Sample Description:AFM TIP: coating testing
Comment:After 3 layer deposition (AI2O3 +SiNx +Al2O3)
Date of Preparation:2024-02-06
Amount of Product:1 tips
Method of Preparation:ALD+ CVD+ALD
Location of Sample:AFM lab
Special Precautions:handling, (small dimension)
State of Sample:after multiplayer deposition : initial characterization
links:[{"lid": "D340", "link": "D340"}]
jasondata:None
```

```
success:1
id:S450
tent:2023-02-14 11:30:47
tcha:2023-04-05 18:03:35
project:S&R
user:davidkordus
type:sample
ancestry:[S443]
descendants:[S650, S1069, S1072]
Name:ZnO/Cu2O NCs on SiO2 (low Zn) (DK20-17-SI)
Preparator:David Kordus
Source:FHI
Sample Description:Cu2O NCs with Zn shell on SiO2
Comment:ZnO/Cu2O NCs (#NC, #CoreShell) on SiO2
- User sample ID: DK20-17-SI
- Mix NCs with SiO2 support (C00007)
- 61.40 mg NCs + 143.26 mg SiO2
Date of Preparation:2020-11-24
Method of Preparation:Mixing and Sonication
Elements:Cu, Zn, Si, O
jasondata:None
links:[{"lid": "179", "link": "D340"}, {"lid": "704", "link": "D799"}, {"lid": "705", "link": "D809"}, {"lid": "706", "link": "D809"}, {"lid": "707", "link": "D809"}, {"lid": "708", "link": "D809"}, {"lid": "709", "link": "D809"}, {"lid": "710", "link": "D809"}, {"lid": "711", "link": "D809"}, {"lid": "712", "link": "D809"}, {"lid": "713", "link": "D809"}, {"lid": "714", "link": "D809"}, {"lid": "715", "link": "D809"}, {"lid": "716", "link": "D809"}, {"lid": "717", "link": "D809"}, {"lid": "718", "link": "D809"}, {"lid": "719", "link": "D809"}, {"lid": "720", "link": "D809"}, {"lid": "721", "link": "D809"}, {"lid": "722", "link": "D809"}, {"lid": "723", "link": "D809"}, {"lid": "724", "link": "D809"}, {"lid": "725", "link": "D809"}, {"lid": "726", "link": "D809"}, {"lid": "727", "link": "D809"}, {"lid": "728", "link": "D809"}, {"lid": "729", "link": "D809"}, {"lid": "730", "link": "D809"}, {"lid": "731", "link": "D809"}, {"lid": "732", "link": "D809"}, {"lid": "733", "link": "D809"}, 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```



EXAMPLE 2: CUSTOM ARCHIVE SEARCH WEB APP

Demonstration Project

Building a custom web site in 2 days
with Python & Flask

What it does:

Graphical web app for searching, running
locally on your laptop.

→ **Searching**

Why?

Built in functionalities sometimes not sufficient

→ **Custom functionalities**

Welcome to the Archive Scraper!

Please enter the URL of your archive.

Please enter your username.

Please enter your password.

submit

<https://gitlab.fhi.mpg.de/beinlich/archive-scraper>
(register first)

Interested in using it? Get in touch!



EXAMPLE 2: CUSTOM ARCHIVE SEARCH WEB APP

Demonstration Project

Building a custom web site in 2 days
with Python & Flask

***A simple & fast way to create a
Graphical App***

Other use cases:

Automatized:

- plot generation,
- report generation,
- file conversion,
- ...

Welcome to the Archive Scraper!

Please enter the URL of your archive.

Please enter your username.

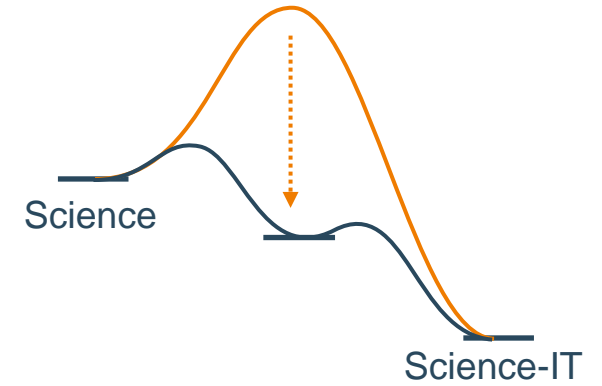
Please enter your password.

<https://gitlab.fhi.mpg.de/beinlich/archive-scraper>
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PYTHON SCRIPTING AND SMALL SERVICES



Advice on how to tackle IT problems

Help with programming

- Python
- Other

What the PP&B can do for you

Help with / provide micro services

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

Help with existing services

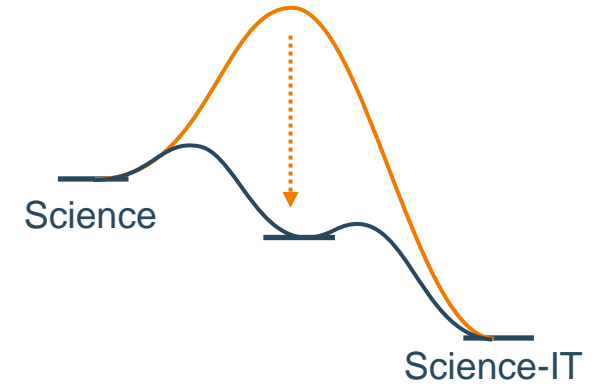
- Archive
- EPICS
- Storage
- ...

Help with script sharing

- GIT



PYTHON SCRIPTING AND SMALL SERVICES



Help with programming

- Python
- Other

Advice on how to tackle IT problems

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Help with existing services

- Archive
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- ...

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!)

GitLab Enterprise Edition

Username or primary email
MyFHusername

Password
.....
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<https://gitlab.fhi.mpg.de>
(register first)



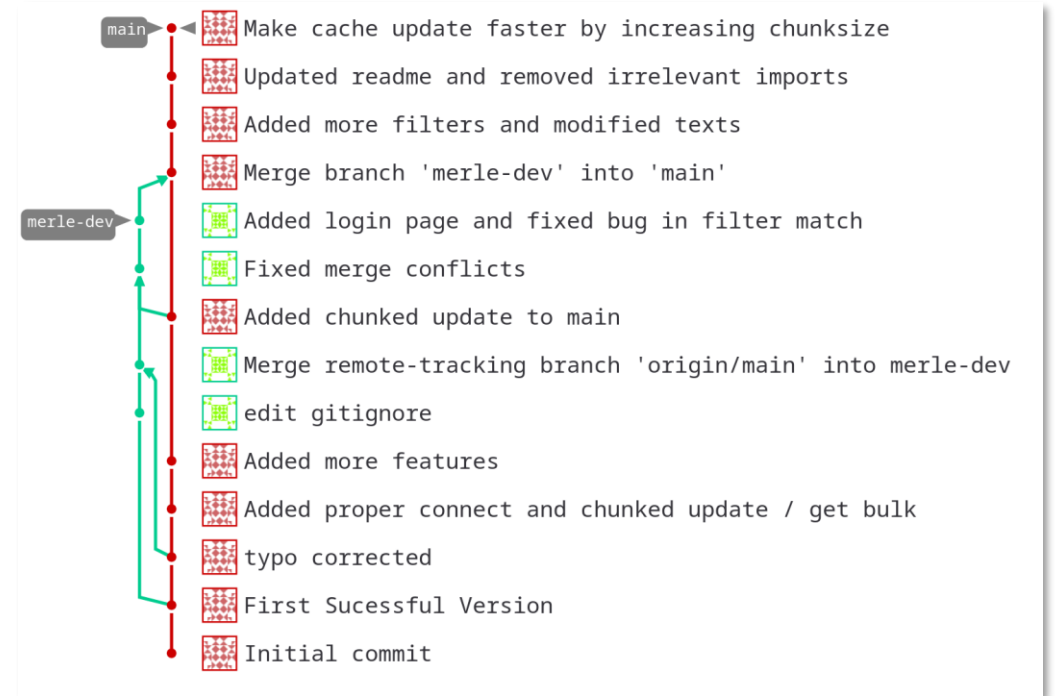
SHARING & COLLECTING ANALYSIS PROCEDURES - GIT

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

COMPLEMENTING EXPERIMENTS WITH SIMULATIONS

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

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

Kinetic Modeling

- Micro Kinetic Modeling
- Kinetic Monte Carlo ...

Large Analyses

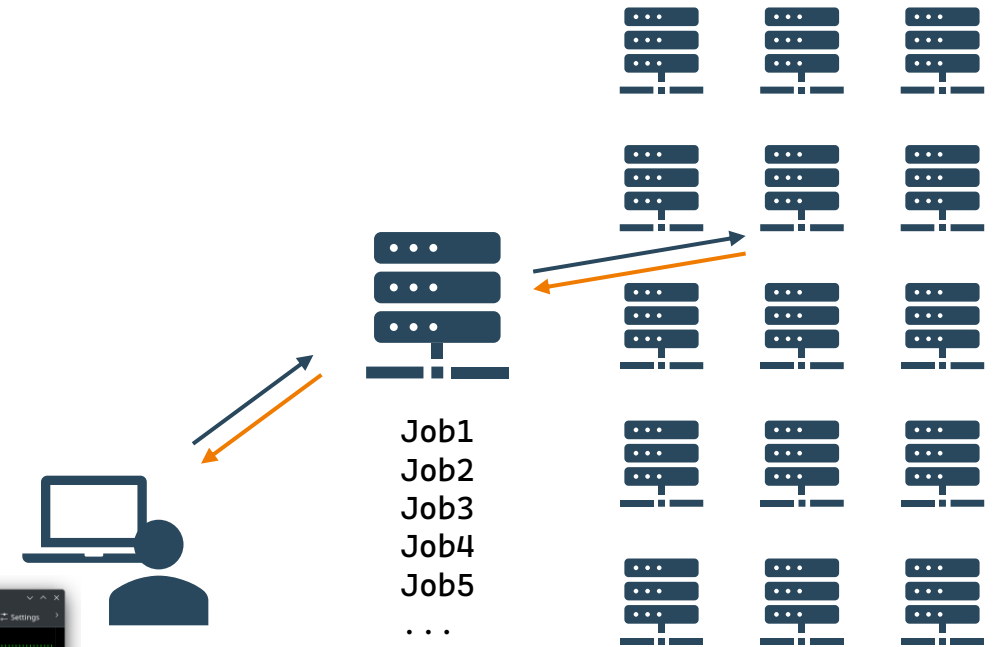
Resource intensive scripts and programs

AI Training

Anything that requires more than a desktop PC



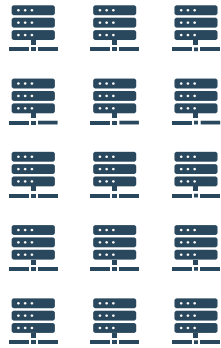
<https://doku.lrz.de/supermuc-ng-10745965.html>



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

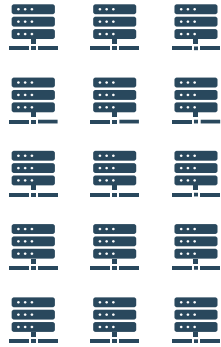
Juwels (JSC)

- >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

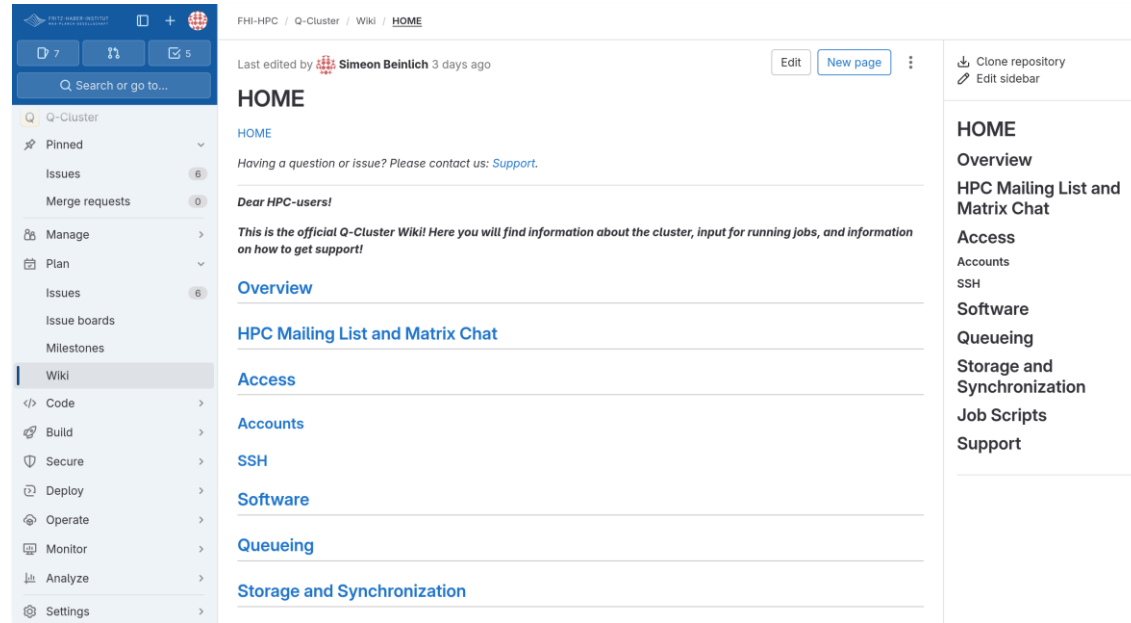
AC

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?

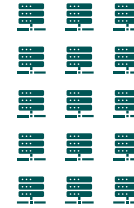
Support?



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	Scheduler	SLURM
CentOS (Linux)	Operating System	SUSE Enterprise (Linux)
RocksCluster	Cluster Setup	-



SUMMARY

Challenges and Pathways in Scientific IT

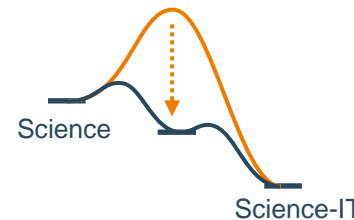
- More (complex) data & setups + More requirements
→ Suitable Infrastructure and Automation
- **From Repetitive & Local to Automatized & Connected**
- Joint approach to tackle challenges
- **From manual to scripted analyses (where possible)**



THANK YOU!

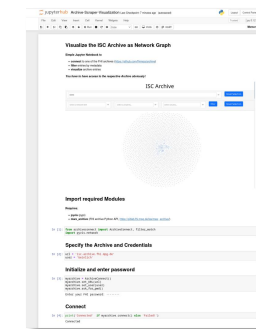
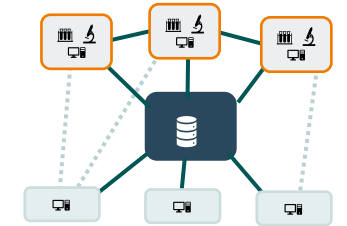
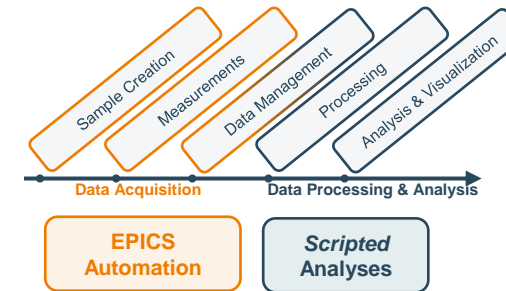
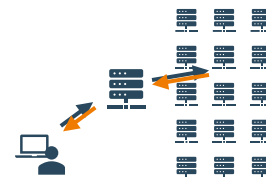
Role of PP&B

- Focus on Science IT
- More support and scientific services



HPC at FHI

- More support
- Less maintenance and administration



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Please enter your username.

Please enter your password.

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archive-visualization

archive-scraper

Need something similar? Get in touch!