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MAX-PLANCK-GESELLSCHAFT

Forschungsdatenmanagement

Von der Datenaufnahme bis zum Laborbuch
(Am Beispiel der IT am Fritz-Haber-Institut)

19. April 2018, Heinz Junkes

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Forschungsdatenmanagement

- Konzept muss bei der Datenaufnahme beginnen.
- Nicht erst, wenn Daten *irgendwie* vorhanden sind.
  - Wo kommen die Daten her?
  - Wie wurde damit bisher umgegangen?
  - Metadaten? Nachvollziehbar? Integrität? Umgebungsparameter?

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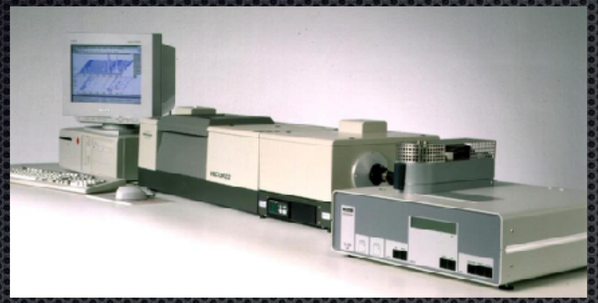

```
./Masters/2016/04/08:
total 0
drwxr-xr-x  1246 heinz  staff  39872 Aug 24  2016 20160408-154156
drwxr-xr-x   415 heinz  staff  13280 Aug 24  2016 20160408-160650

./Masters/2016/04/08/20160408-154156:
total 5871728
-rw-------@ 1 heinz  staff  2078667 Mar 15  2016 IMG_3978.JPG
-rw-------@ 1 heinz  staff  2030296 Mar 15  2016 IMG_3979.JPG
-rw-------@ 1 heinz  staff  2074129 Mar 15  2016 IMG_3980.JPG
-rw-------@ 1 heinz  staff  2395040 Mar 18  2016 IMG_3981.JPG
-rw-------@ 1 heinz  staff  2496720 Mar 18  2016 IMG_3982.JPG
-rw-------@ 1 heinz  staff  2449278 Mar 18  2016 IMG_3983.JPG
```

Oft (meist) black-box Systeme.

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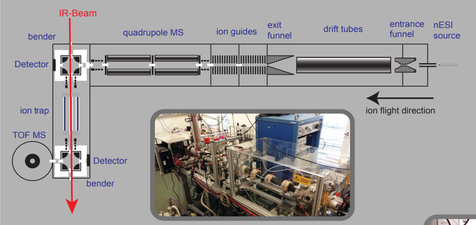

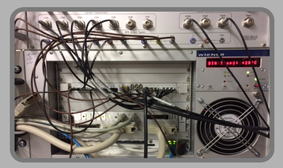

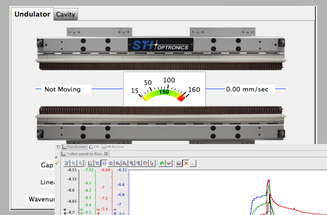

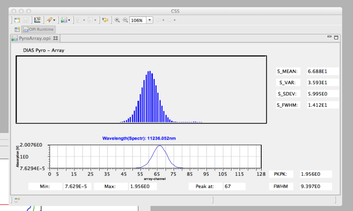

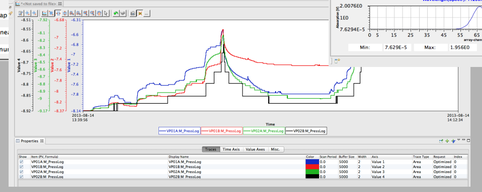

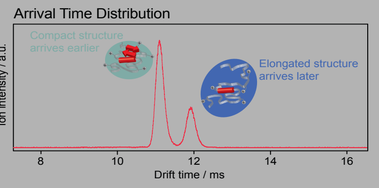

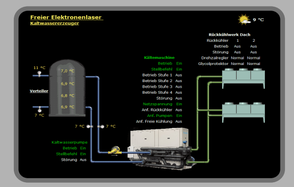

ptp2
appl. tag

Dokumentation u. API Beschreibung RTD	Versionskontrolle OS u. Anwendung mercurial / git	Archiver archiverAppliance	Elektr. Laborbuch olog, elog (labforder)	save/restore channelfinder

epics-framework
http://epics-controls.org

IT Struktur am FHI

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EPICS record reference
https://wiki-ext.aps.anl.gov/epics

```
epics@felgate:~$ cainfo AGRAJAG:pyroArray
AGRAJAG:pyroArray
    State:            connected
    Host:             agrajag:5064
    Access:           read, write
    Native data type: DBF_DOUBLE
    Request type:     DBR_DOUBLE
    Element count:    130
```

```
epics@felgate:~$ caget -a AGRAJAG:pyroArray
AGRAJAG:pyroArray 2018-04-17 16:16:55.073681 130 0.0162506 0.0115204 0.0107574 ...
0.0157928 0.0163269 0.0113678 0.016861 0.0156403 0.0161743 0.0211334 0.0147247 0.012207 0 681
```

```
epics> dbpr AGRAJAG:pyroArray,4
ACKS: NO_ALARM      ACKT: YES          APST: Always          ASG:
ASP: (nil)          BKPT: 00           BPTR: 0x805a8c8       BUSY: 0
DESC:               DISA: 0            DISP: 0               DISS: NO_ALARM
DISV: 42            DPVT: 0x805ace0    DSET: 0x80502b8       DTYP: diasPyro
EGU: V              EVNT: 0            FLNK:DB_LINK AGRAJAG:shotNr
FTVL: DOUBLE        HASH: 0            HOPR: 2.5             INP:CONSTANT 20000
LCNT: 0             LOPR: 0            LSET: 0x805af90
MLIS: 88 9b 0d 08 b0 9b 0d 08 0a 00 00 00                    MLOK: b0 a8 05 08
MPST: Always        NAME: AGRAJAG:pyroArray                  NELM: 130
NORD: 130           NSEV: NO_ALARM     NSTA: NO_ALARM        PACT: 0
PHAS: 0             PINI: NO           PPN: (nil)            PPNR: (nil)
PREC: 4             PRIO: LOW          PROC: 0               PUTF: 0
RARM: 0             RDES: 0x809d868    RPRO: 0               RSET: 0xb7f7db60
SCAN: I/O Intr      SDIS:CONSTANT      SEVR: NO_ALARM        SIML:CONSTANT
SIMM: NO            SIMS: NO_ALARM     SIOL:CONSTANT         SPVT: 0x805b7b8
STAT: NO_ALARM      TIME: 2018-04-17 16:22:11.476845000      TPRO: 0
TSE: -2             TSEL:CONSTANT 42   UDF: 0                VAL: (nil)
```

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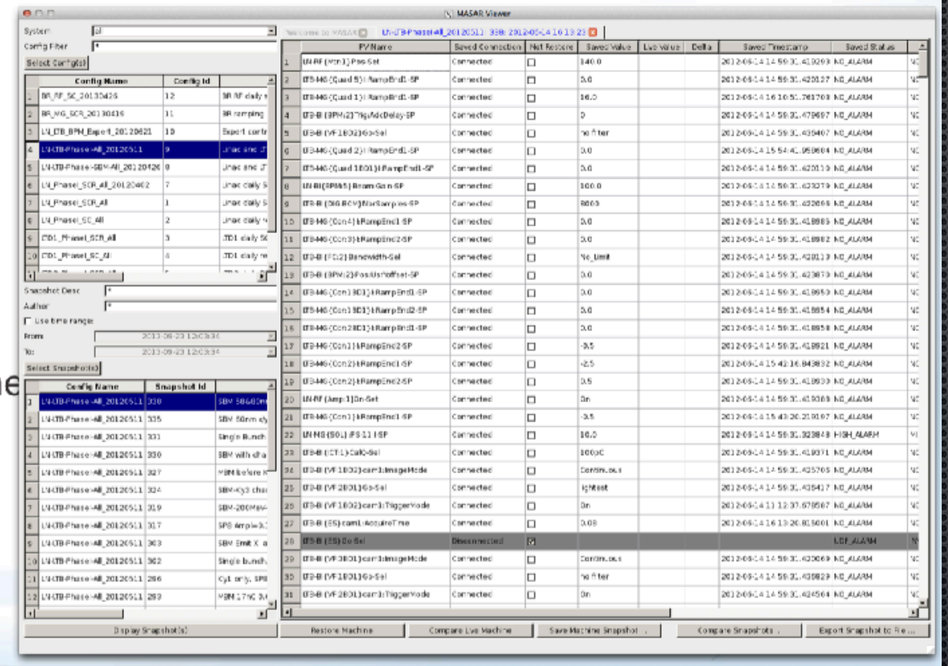
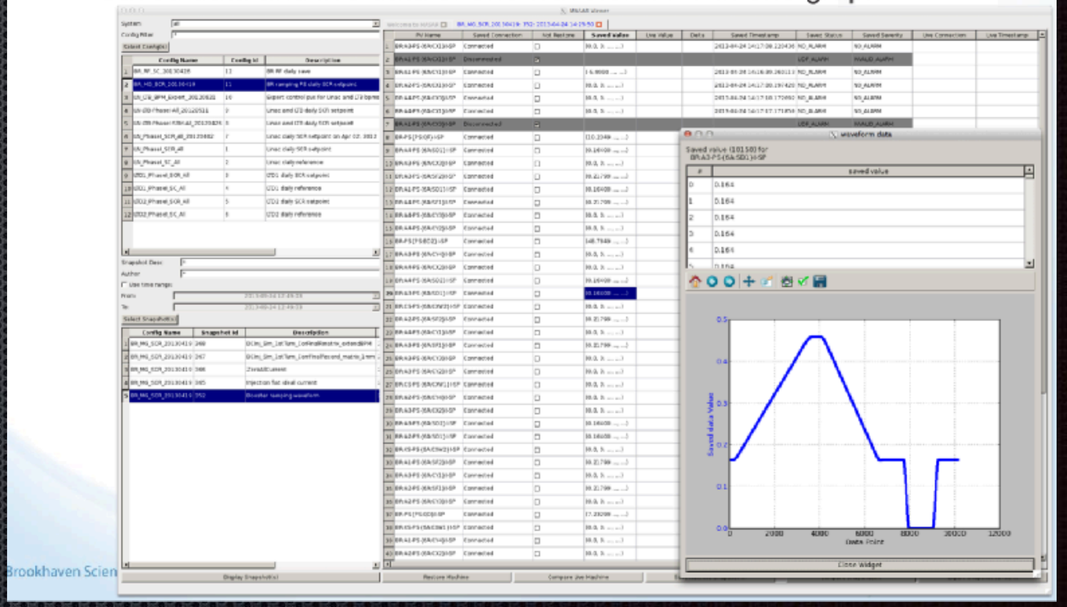
- API for scripting environment
  - 7 APIs in Python
- PyQt UI
  - Based on above APIs
  - Browse config
  - Browse event
  - Take snapshot
  - Retrieve data
  - Compare data
  - Restore machine
  - Export data



- Data plot for waveform PV
  - Saved data and live data of one waveform PV in one graph



MASAR: save&restore (https://github.com/epics-base/masarService)

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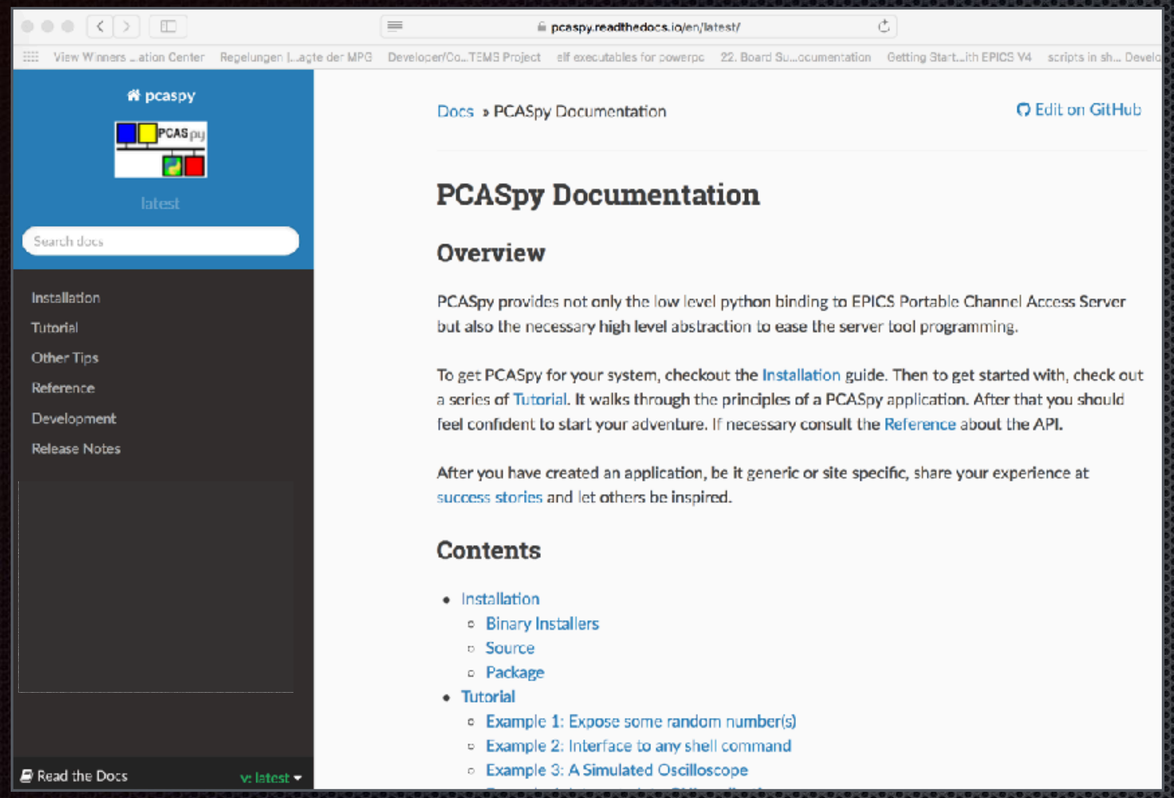
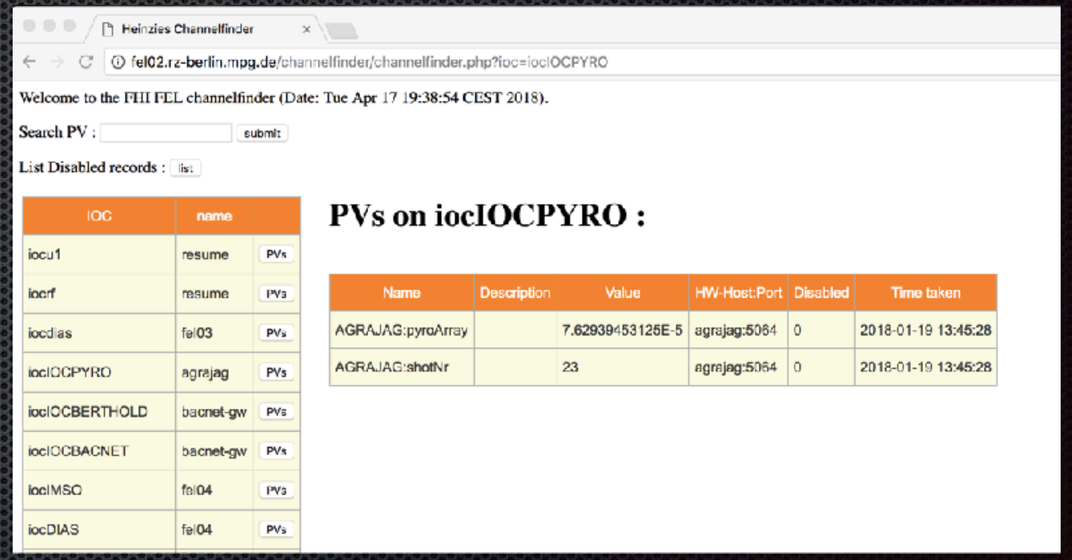


DirectoryService channelfinder (https://github.com/ChannelFinder)



Read the docs (https://readthedocs.org) auf eigener Server-Instanz

Auch innerhalb der MPG verfügbar: https://github.molgen.mpg.de

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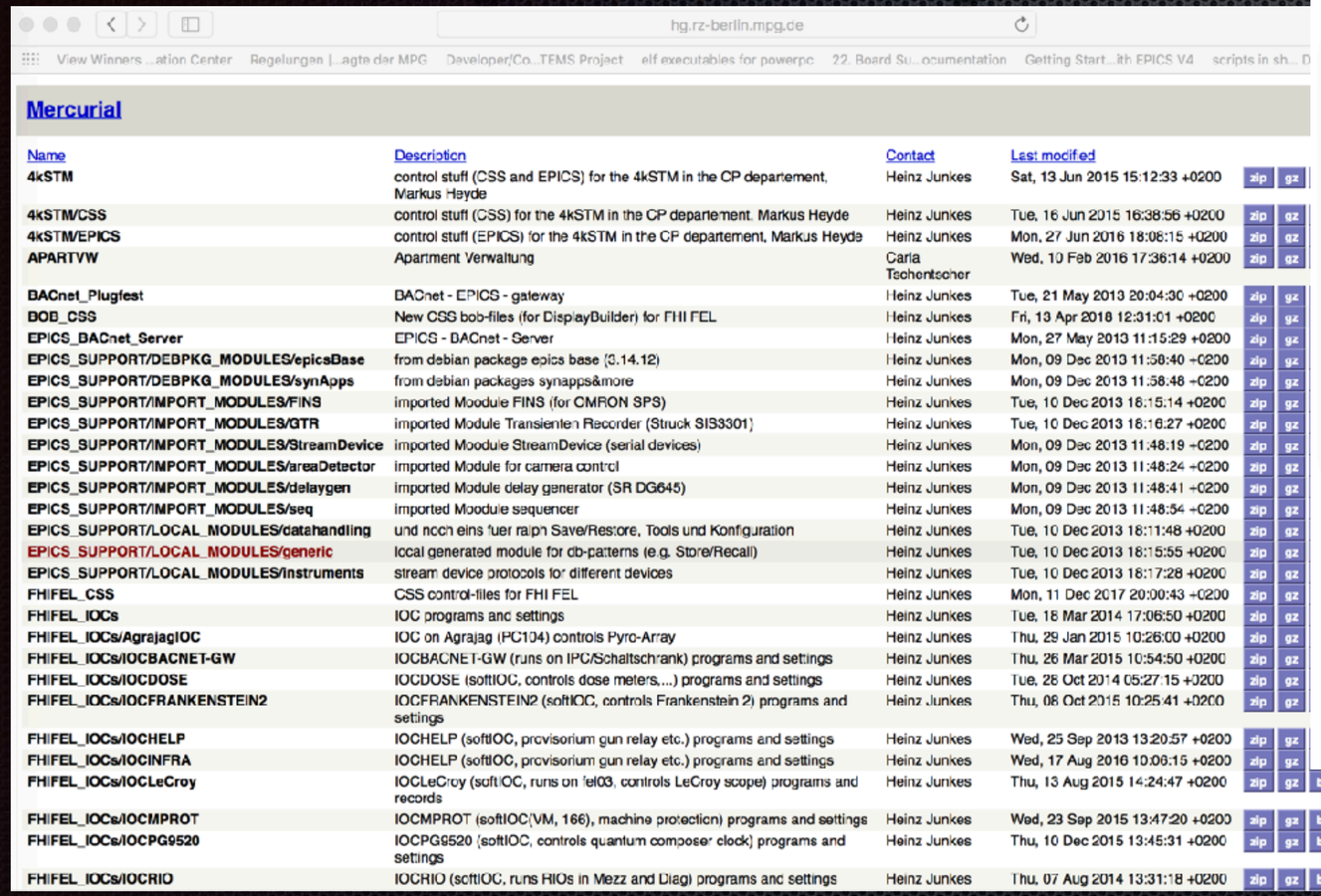
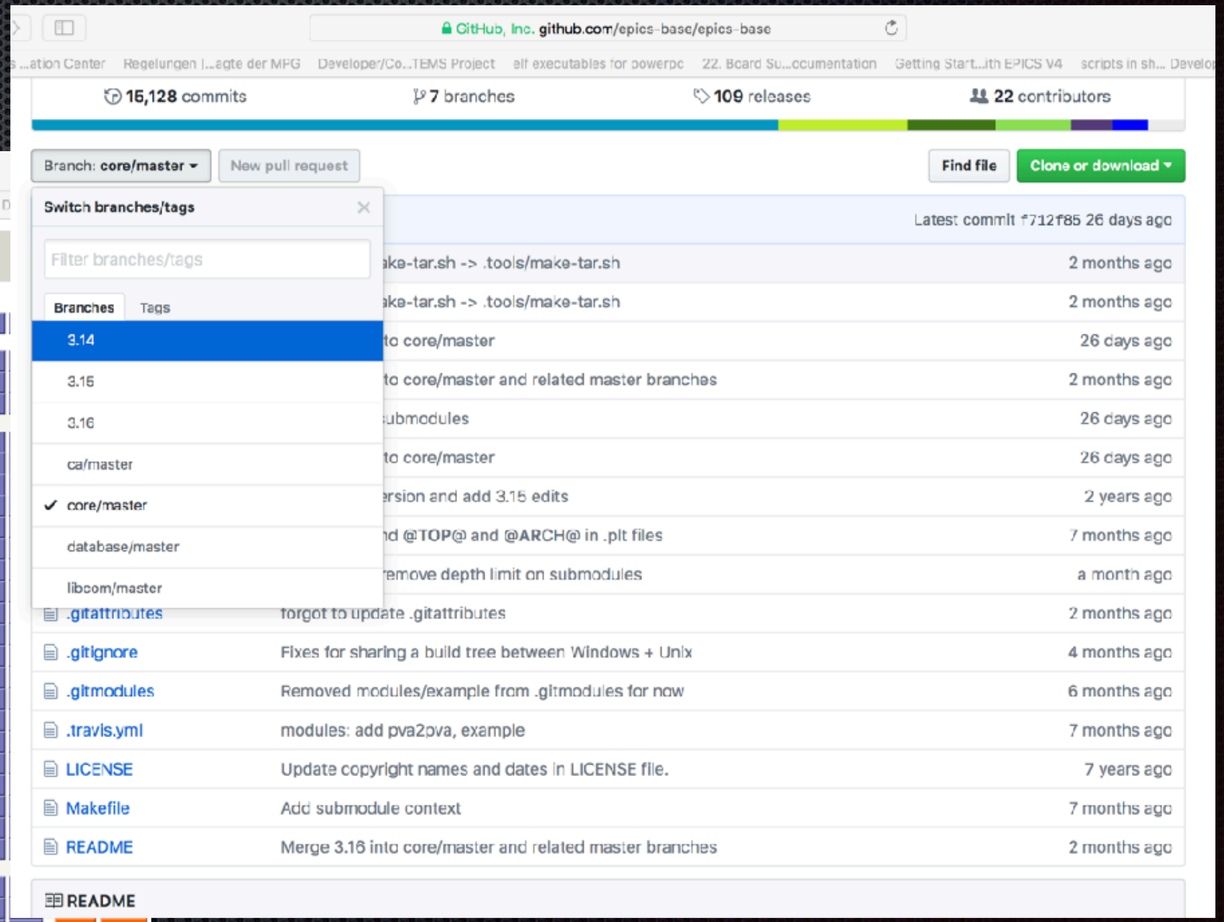
Versionskontrolle (incl. Konfiguration und Algorithmen)



mercurial (https://www.mercurial-scm.org)



git (https://github.com)

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Archivierung

- Monitoring aller Prozessvariablen (PV) und Speicherung bei Änderungen
- Cluster fähig (Appliance)
- Millionen von PVs, incl. Waveforms, ND-Arrays etc.
- Am FHI genutztes System: EPICS ArchiverAppliance

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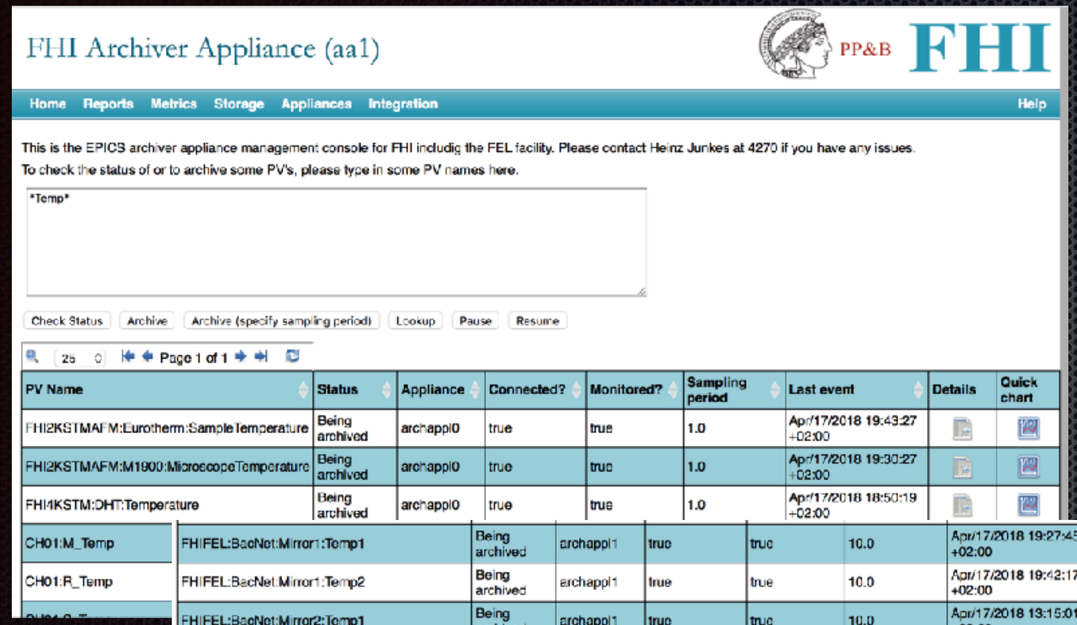

FHI Archiver Appliance (aa1)

PP&B FHI

Home Reports Metrics Storage Appliances Integration Help

This is the EPICS archiver appliance management console for FHI includig the FEL facility. Please contact Heinz Junkes at 4270 if you have any issues.
To check the status of or to archive some PV's, please type in some PV names here.

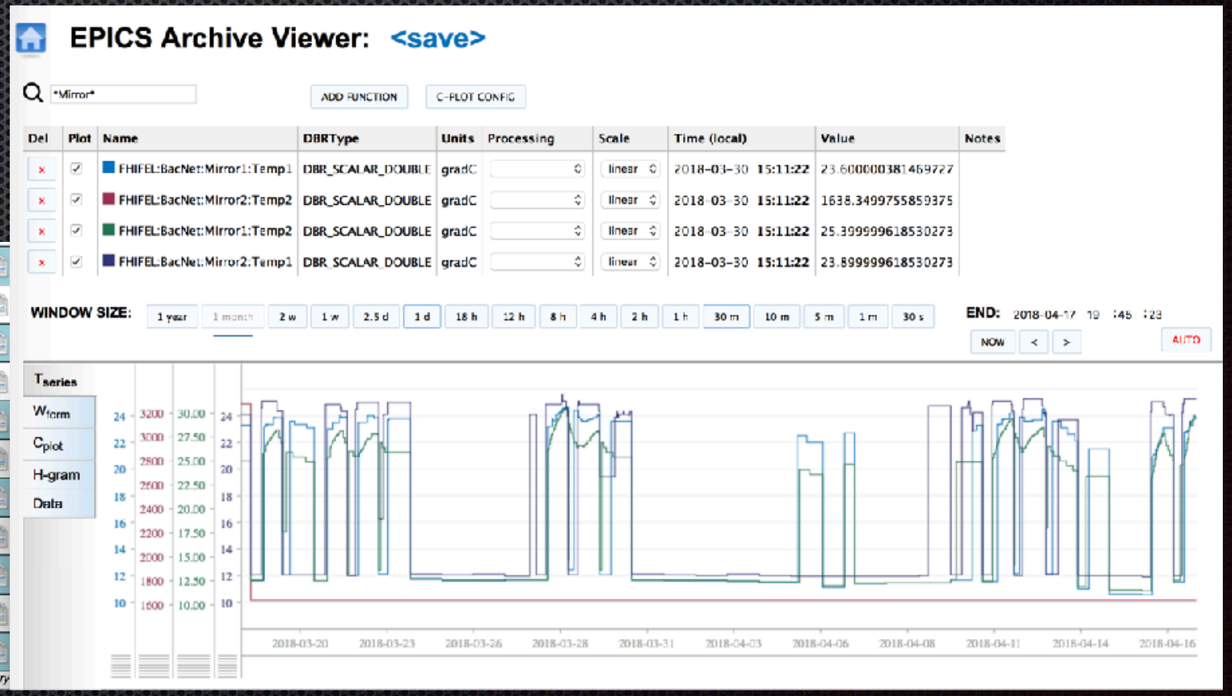
Temp

Check Status | Archive | Archive (specify sampling period) | Lookup | Pause | Resume

25 Page 1 of 1

PV Name	Status	Appliance	Connected?	Monitored?	Sampling period	Last event	Details	Quick chart
FHI2KSTMAFM:Eurotherm:SampleTemperature	Being archived	archappl0	true	true	1.0	Apr/17/2018 19:43:27 +02:00		
FHI2KSTMAFM:M1900:MicroscopeTemperature	Being archived	archappl0	true	true	1.0	Apr/17/2018 19:30:27 +02:00		
FHI4KSTM:DHT:Temperature	Being archived	archappl0	true	true	1.0	Apr/17/2018 18:50:19 +02:00		
CH01:M_Temp	FHIFEL:BacNet:Mirror1:Temp1	Being archived	archappl1	true	true	10.0	Apr/17/2018 19:27:45 +02:00	
CH01:R_Temp	FHIFEL:BacNet:Mirror1:Temp2	Being archived	archappl1	true	true	10.0	Apr/17/2018 19:42:17 +02:00	
	FHIFEL:BacNet:Mirror2:Temp1	Being archived	archappl1	true	true	10.0	Apr/17/2018 13:15:01 +02:00	
	FHIFEL:BacNet:Mirror2:Temp2	Being archived	archappl1	true	true	10.0	Apr/17/2018 01:59:50 +02:00	
	FHIFEL:BacNet:RLT:TempBunker_1	Being archived	archappl1	true	true	120.0	Apr/17/2018 18:35:48 +02:00	
	FHIFEL:BacNet:RLT:TempBunker_2	Being archived	archappl1	true	true	120.0	Apr/17/2018 19:29:48 +02:00	
	FHIFEL:BacNet:RLT:TempBunker_3	Being archived	archappl1	true	true	120.0	Apr/17/2018 19:29:48 +02:00	
	FHIFEL:BacNet:RLT:TempBunker_4	Being archived	archappl1	true	true	120.0	Apr/17/2018 19:41:48 +02:00	
	FHIFEL:TV301SF1:PumpTemperature	Being archived	archappl1	true	true	60.0	Apr/17/2018 19:42:31 +02:00	
	FHIFEL:TV301SF2:PumpTemperature	Being archived	archappl1	true	true	60.0	Apr/17/2018 19:35:41 +02:00	
	FHIFEL:TV301SF3:PumpTemperature	Being archived	archappl1	true	true	60.0	Apr/17/2018 19:37:21 +02:00	

EPICS Archiver Appliance Version 0.0.1_SNAPSHOT_16-January


EPICS Archive Viewer: <save>

Mirror ADD FUNCTION C-PLOT CONFIG

Del	Plot	Name	DBRType	Units	Processing	Scale	Time (local)	Value	Notes
x	✓	FHIFEL:BacNet:Mirror1:Temp1	DBR_SCALAR_DOUBLE	gradC		linear	2018-03-30 15:11:22	23.600000381469727	
x	✓	FHIFEL:BacNet:Mirror2:Temp2	DBR_SCALAR_DOUBLE	gradC		linear	2018-03-30 15:11:22	1638.3499755859375	
x	✓	FHIFEL:BacNet:Mirror1:Temp2	DBR_SCALAR_DOUBLE	gradC		linear	2018-03-30 15:11:22	25.399999618530273	
x	✓	FHIFEL:BacNet:Mirror2:Temp1	DBR_SCALAR_DOUBLE	gradC		linear	2018-03-30 15:11:22	23.899999618530273	

WINDOW SIZE: 1 year | 1 month | 2 w | 1 w | 2.5 d | 1 d | 18 h | 12 h | 8 h | 4 h | 2 h | 1 h | 30 m | 10 m | 5 m | 1 m | 30 s

END: 2018-04-17 19 :45 :23 NOW < > AUTO

Tseries | Wform | Cplot | H-gram | Data

https://slacmshankar.github.io/epicsarchiver_docs/

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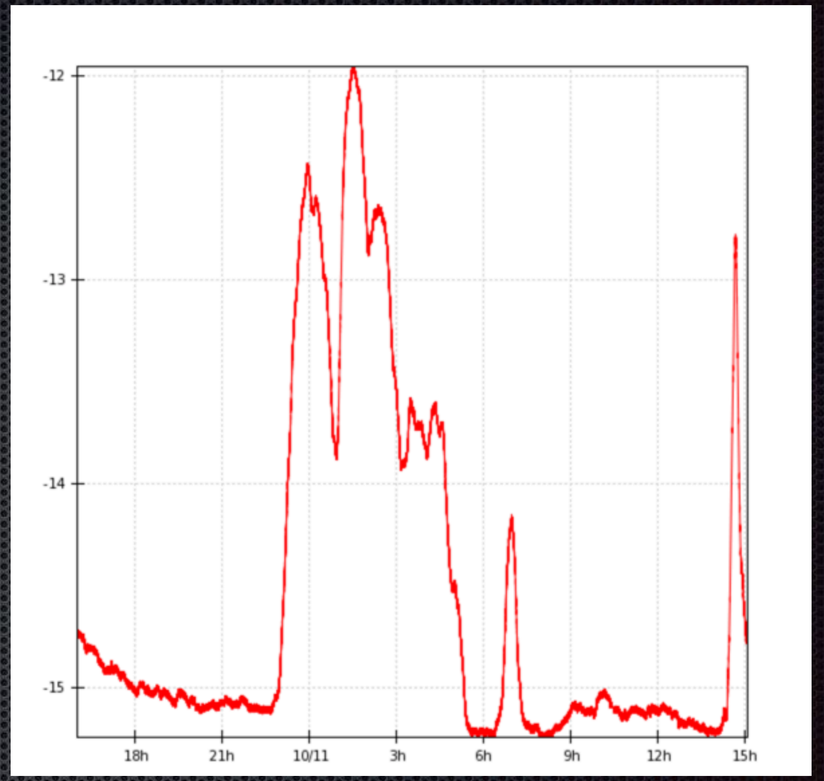
```
import numpy as np
from chaco.shell import *
import urllib2
import json

req = urllib2.urlopen("http://archiver.slac.stanford.edu/retrieval/data/getData.json?pv=test%3Apv%3A123&donotchunk")
data = json.load(req)
secs = [x['secs'] for x in data[0]['data']]
vals = [x['val'] for x in data[0]['data']]
plot(secs, vals, "r-")
xscale('time')
show()
```



archiver retrieval

Retrieving data using other tools

The EPICS Archiver Appliance supports data retrieval in multiple formats/MIME types. These are some of the few formats supported today; more can easily be added as needed.

1. JSON - A generic JSON format that can be easily loaded into most browsers using Javascript.
2. CSV - Can be used for importing into Excel and other spreadsheets.
3. MAT - This is the file format used for interoperating with Matlab.
4. RAW - This is a binary format used by the Archive Viewer and is based on the PB/HTTP protocol.
5. TXT - A simple text format that is often helpful for debugging.
6. SVG - A XML format that can also be used as a SVG element in tools that support this format.

In general, getting data into a tool necessitates construction of a data retrieval URL as the first step. A data retrieval URL looks something like so

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Elektronisches Laborbuch

- Einträge in das Laborbuch müssen automatisiert werden können
- Benötigt Import/Export API (unlimited users, dokumentiert)
- Muss administrierbar, skalierbar und austauschbar sein
- Am FHI genutzte elektronische Laborbücher: olog, elog, (labfolder)

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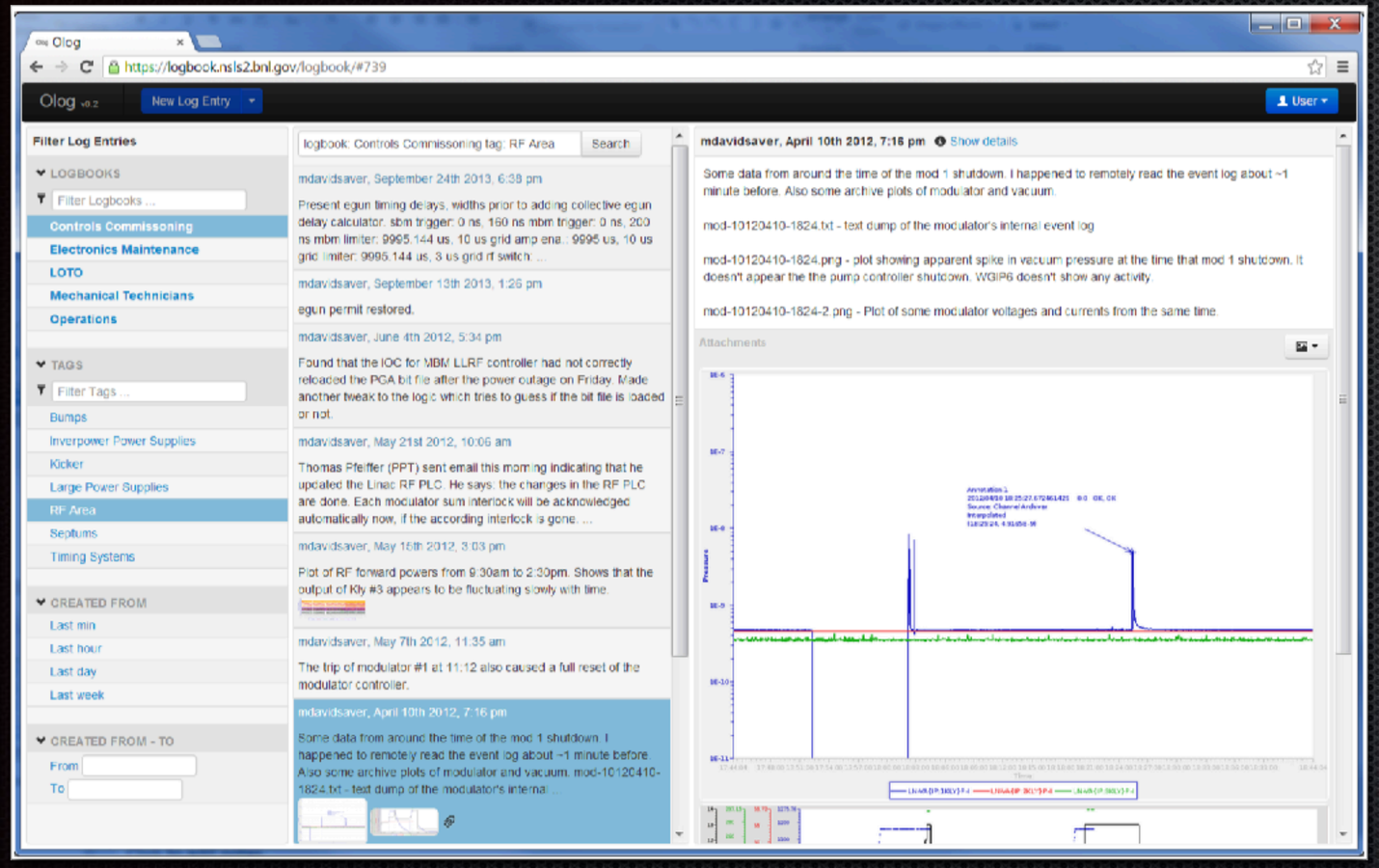
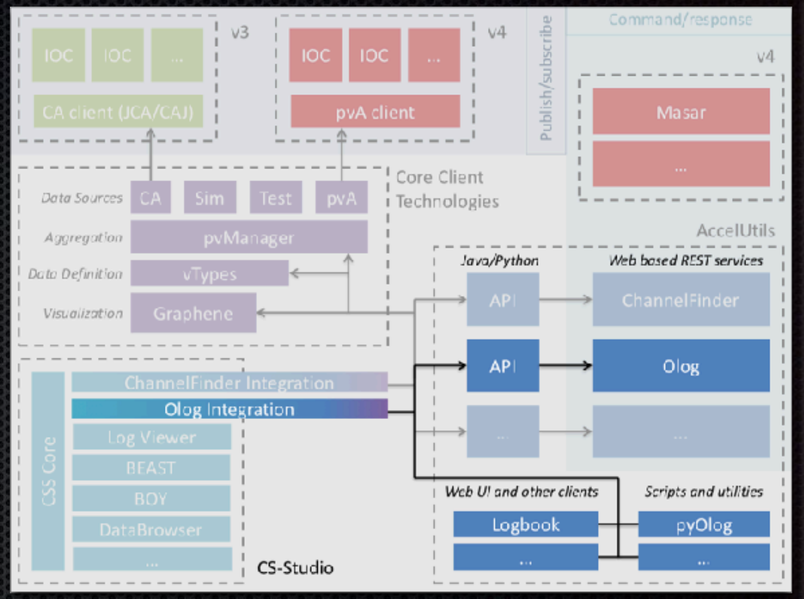


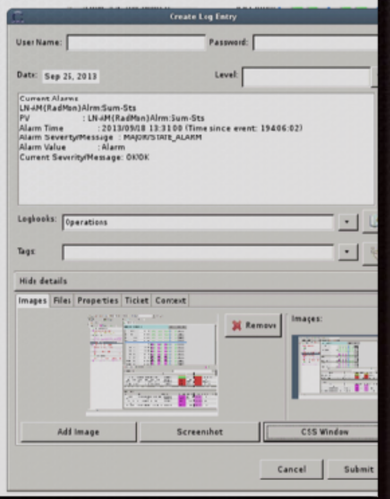


Olog Clients – CS-Studio

Log Entries initialized with application specific information

Alarm server

- PV name
- Alarm status
- Alarm time



Olog: https://github.com/Olog

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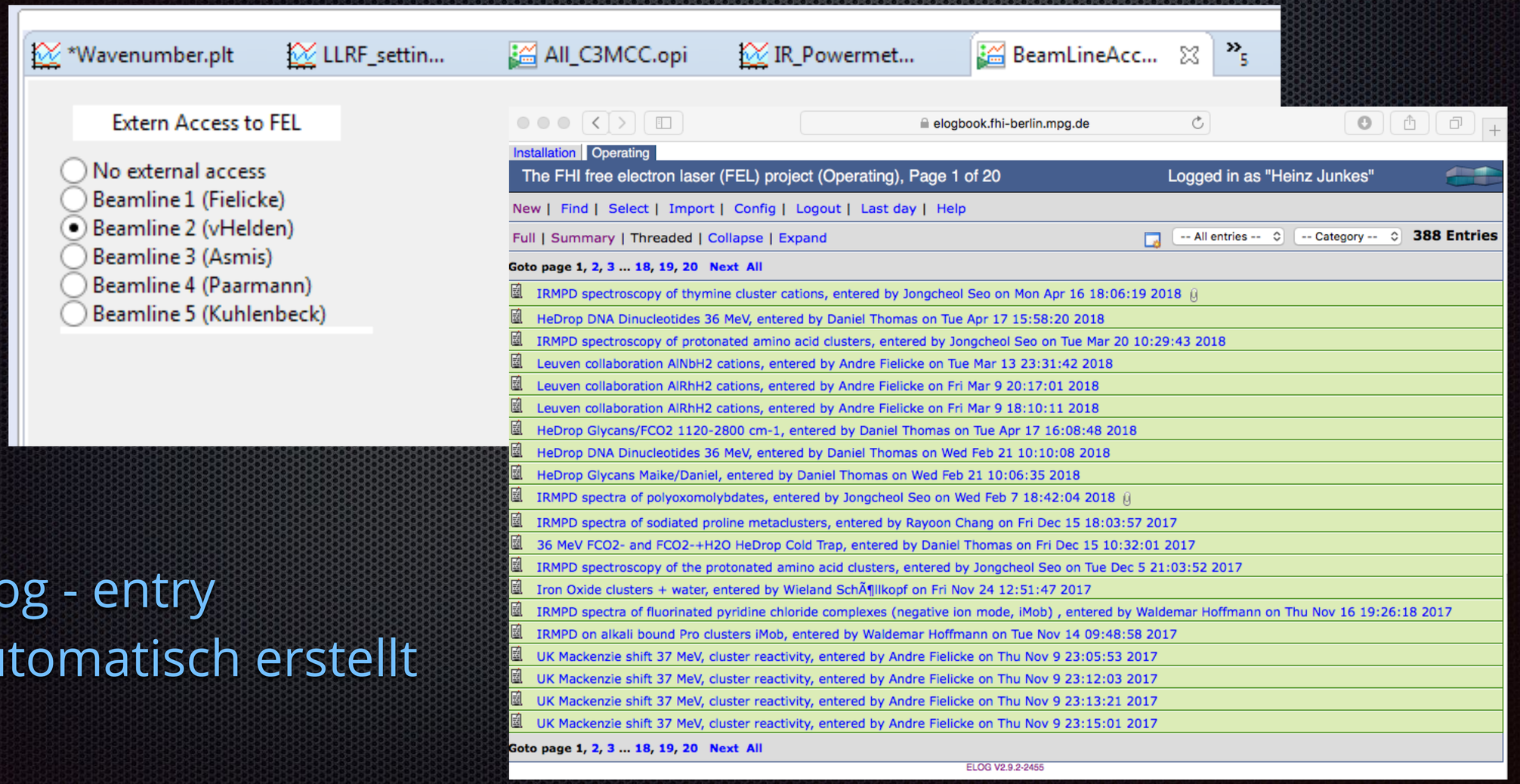

shift - log - entry
wird automatisch erstellt

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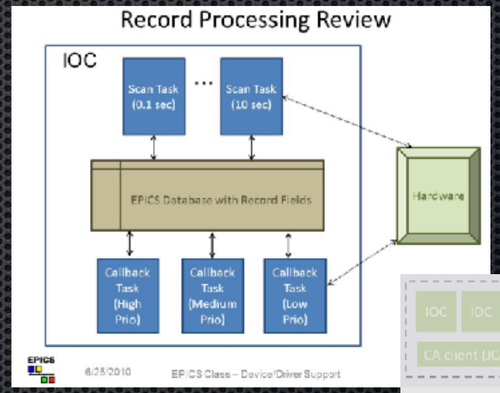
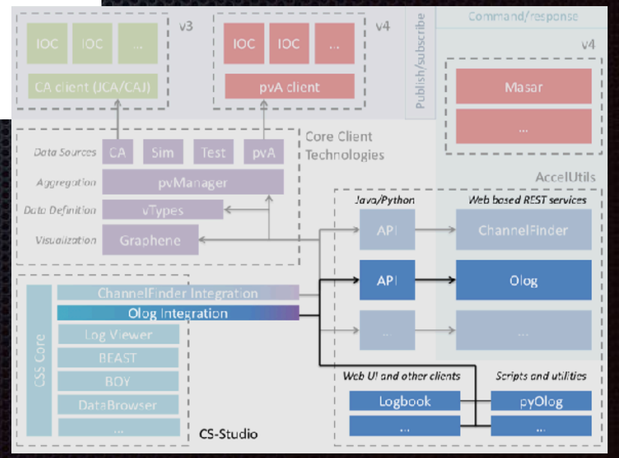
Aus MPDL Forschungsbericht 2017 “Elektronische Laborbücher in der Max-Planck-Gesellschaft” :

“Individuelle Flexibilität ist für die meisten Forschenden essenziell: Da sich die Experimentalanordnungen gerade im Forschungskontext oft ändern sind Systeme, welche auf einen hohen Automatisierungsgrad der Arbeitsabläufe setzen, eher ungeeignet.”
(https://www.mpg.de/10988930/_jb_2017)

- Widerspruch!
  - Durch die Integration der elektronischen Laborbücher in die Datenaufnahme “folgen” die Einträge den Änderungen der Experimentalanordnung





elog Vortrag : http://eln.mpdl.mpg.de/wp-content/uploads/2016/03/ELN_Junkes.pdf

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Labfolder

- Wurde von MPDL zentral beschafft
- Wegen Erscheinungsbild bei den Usern gerne gesehen
- Aussen hui, innen pfui? Keine Export/Import Funktionalität
- Nicht administrierbar, nicht skalierbar, nicht austauschbar
- Wie kommen wir da wieder raus? *Plan B* vorhanden?