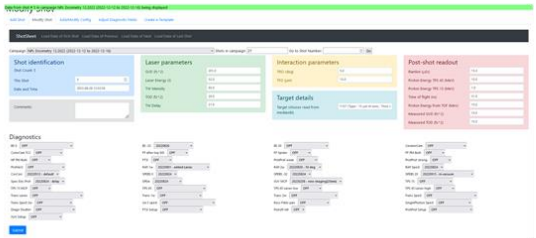
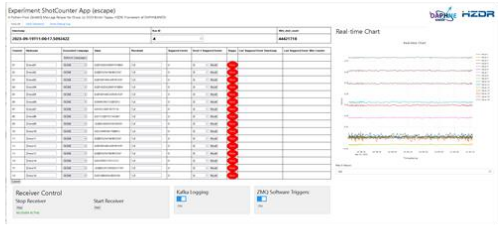
Hosted by: Fwklux9:8080, 8082

Shotsheet [ions] https://149.220.59.21:8080/
and [electrons] https://149.220.59.21:8082/



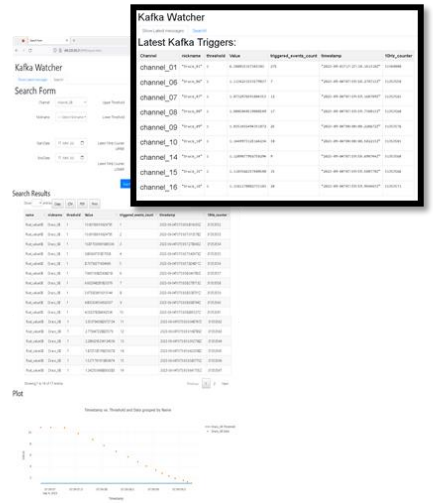
Fwk573:8888

ZeroMQ Relay
http://149.220.59.31:8888/



Fwklux9:9999

Kafka Receiver and MongoDB Relay
https://149.220.59.21:9999/



SciCat Upload Tools

Advancing Research Data Management with Python-Flask Applications

Helmholtz Metadata Collaboration | Conference 2023

Helmholtz-Zentrum Dresden-Rossendorf · FWKT · Dr. Kristin Tippey · k.tippey@hzdr.de · www.hzdr.de

Problem Statement

PROBLEM STATEMENT

Data acquisition (DAQ) systems continue to advance in power, but manual data input will remain required as experiments necessarily check for the unforeseen. Researchers often use electronic lab books or fallback solutions like Excel or Google Docs to record actions and events, highlighting the need for an **intuitive interface that enables live- and post-processing while remaining linkable to DAQ systems**.

CHALLENGES

A major challenge lies in the **dynamic nature of the incoming information**, rendering fixed-structure databases like SQL impractical. What can we read in automatically? What manual input do we need?

APPROACH

To tackle this issue, we have developed **intuitive Python-Flask applications** that harness the inherent flexibility of document-based databases, particularly MongoDB, for storing curated and query-ready data. Although these applications were initially tailored for the laser-particle acceleration group at HZDR as part of the DAHPNE4NFDI project, the intention is to generalize their utility.

Enter Flask WebApps

Why Flask?

Flask is a micro web framework written in Python.

Like Django but simpler, and less strictly structured.

Why WebApps?

Available anywhere.

What can you do with them?

Turns out, a lot.

- Configurable forms
- Configurable selections
- Search and changeability

Enter Flask WebApps

1. ShotSheet [ions, electrons]

Need: Issues extending and FAIRizing current ShotSheet

- Facilitates manual data entry during experiments via a database form
- Can be easily – and on-the-fly – changed and allows also to store the DAQ configuration per entry
- Choices can be pre-configured or pulled from sources like a MediaWiki lab documentation system
- Entries are directly written to a MongoDB

2. ZeroMQ Relayer

Need: No existing dedicated Draco counter for counting triggered shots

- Extracts metadata from the experiment's drive laser (via zeroMQ) and forwards this in real-time to visualization app and to Kafka
- Enables harmonized metadata like ID's and timestamps, either appended to data as well as logged for post-hoc reconstruction

3. KafkaWatcher

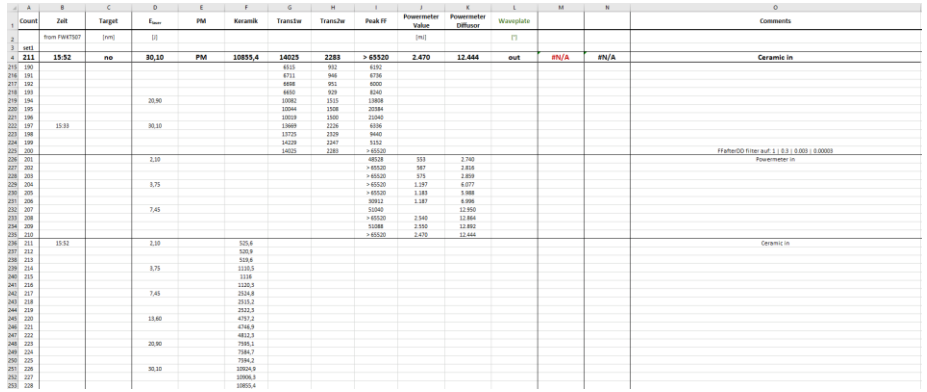
Need: Receive/monitor new Draco counter

- Functioning as an intermediary, this app receives data from the Relayer and publishes it to MongoDB
- Flask-SocketIO is used for real-time reception of Kafka messages

Shotsheet: Evolution of the Shotsheet

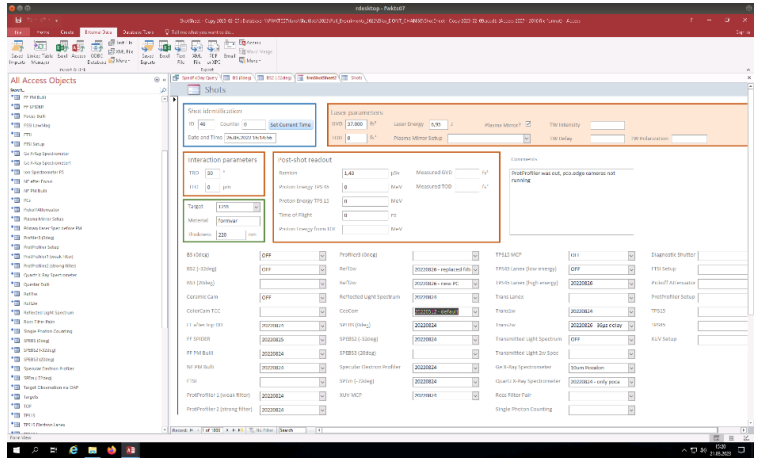
Started as Excel

- Limitations … often all the interesting diagnostics ended up in the first column of Comments
- Difficult to catalogue post-experiment
- Not very FAIR



Moved to Microsoft Access

- Better tracking of data corresponding to individual shots
- Slow loading
- Issues accessing/exporting data
- More FAIR but still not really FAIR
- Lately limitations on number of diagnostics has accelerated the need for a new method



Shotsheet: A Python-Flask WebApp with a MongoDB Backend

Newest Shotsheet, Built separate version for Ions and Electrons

Why????

Python Physicists like python. I already had a decent grasp on Python so it was the least extra work to getting started

Flask Adaptable and relatively simple microframe-work with wide range of supported features

MongoDB NoSQL document-based database

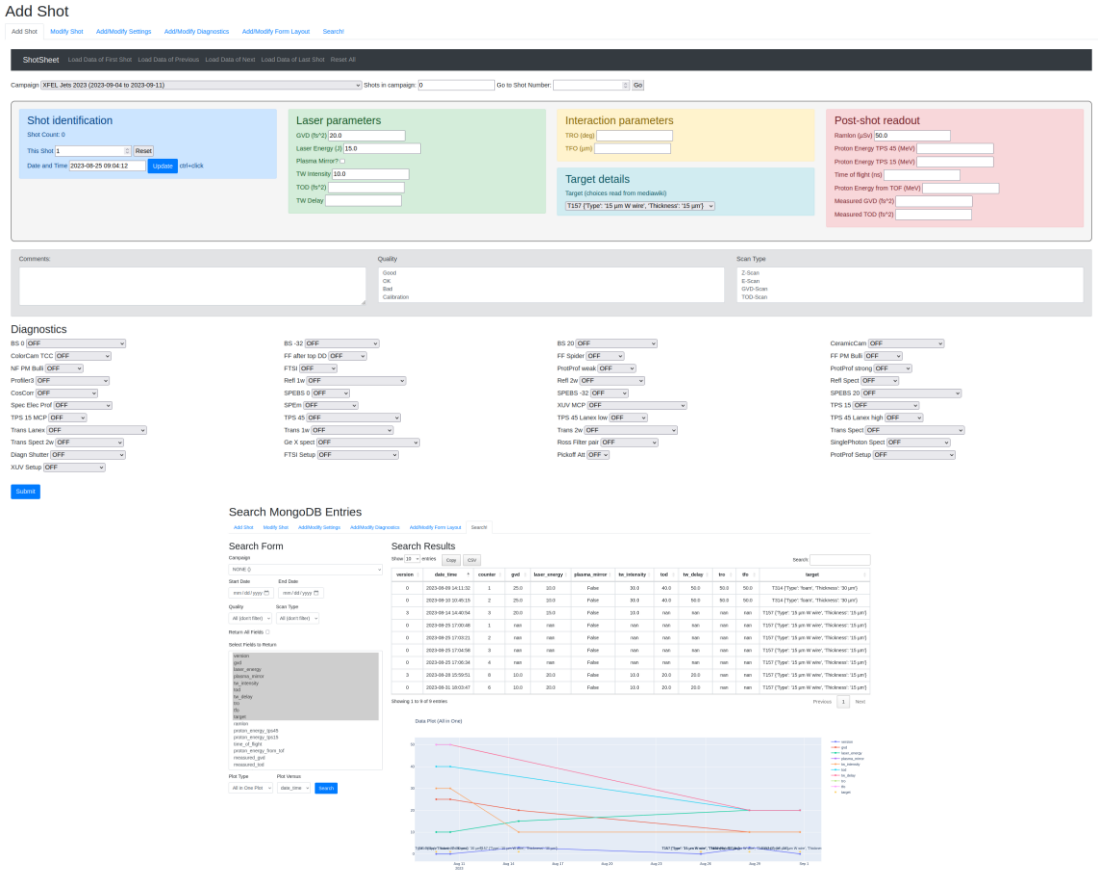
Other supporting Elements

WTForms form validation

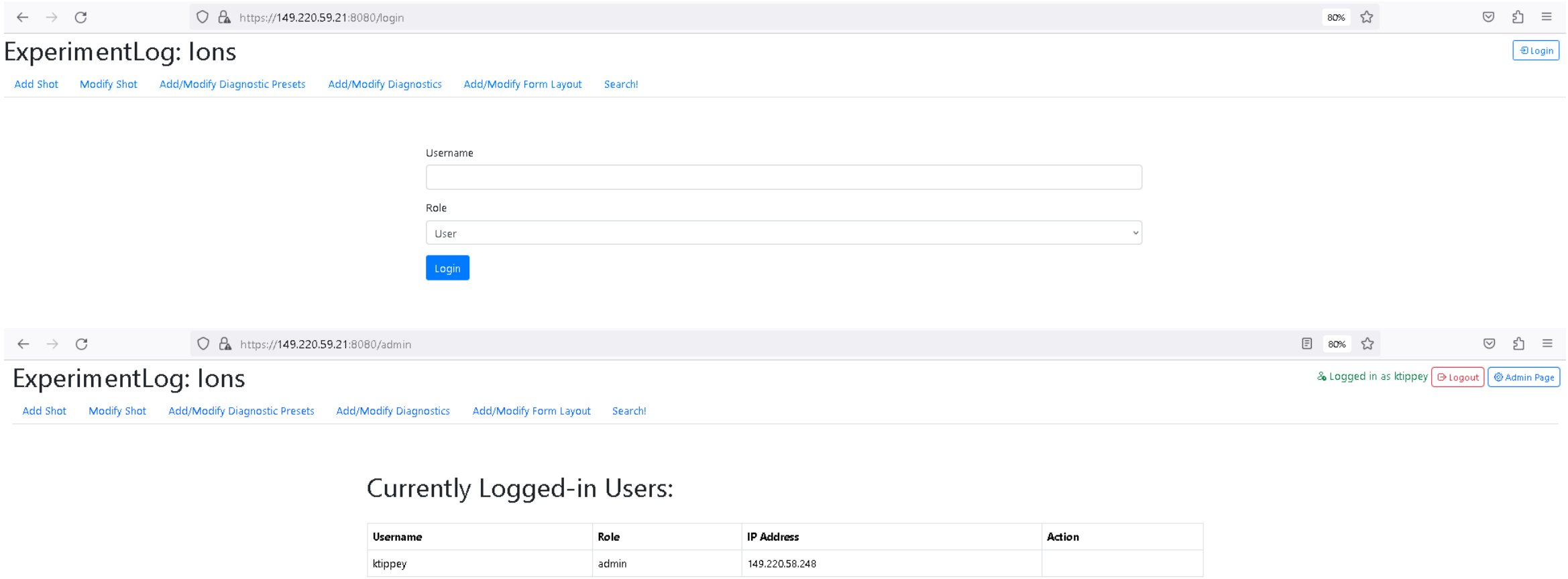
Javascript dynamic features

Jinja2 template management

Bootstrap clean consistent form layouts



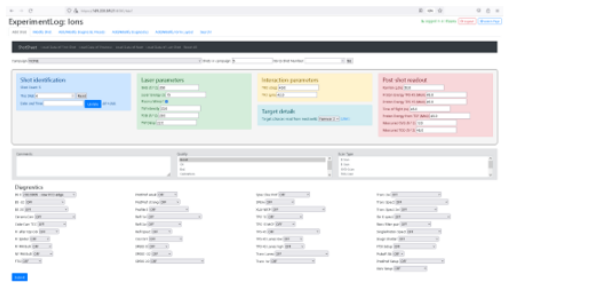
Working on basic user tracking for access to Add/ModifyShot [User] and RemoteUserLogout [Admin] pages



Shotsheet [ions]: The different tabs

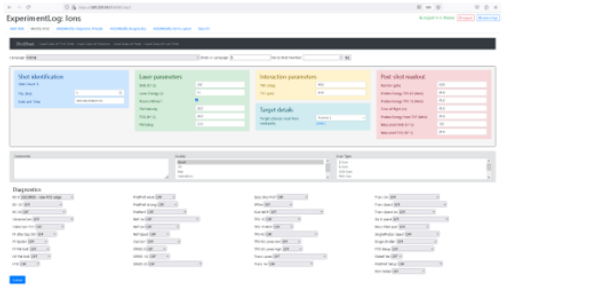
Outline

Add Shot



7

Modify Shot

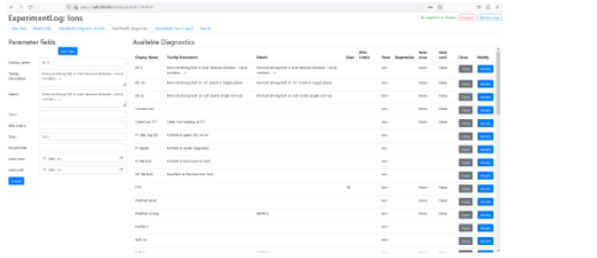


8

Add/Modify Diagnostic Presets

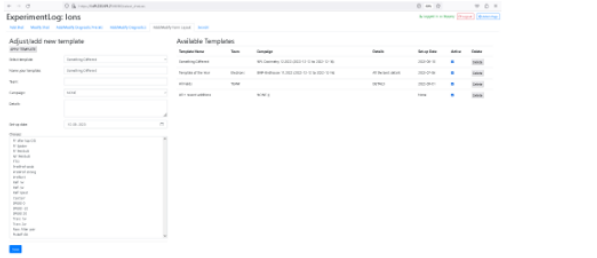
9

Ad/Modify Diagnostics



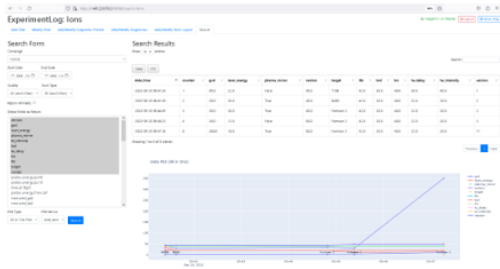
10

Add/Modify Form Layout



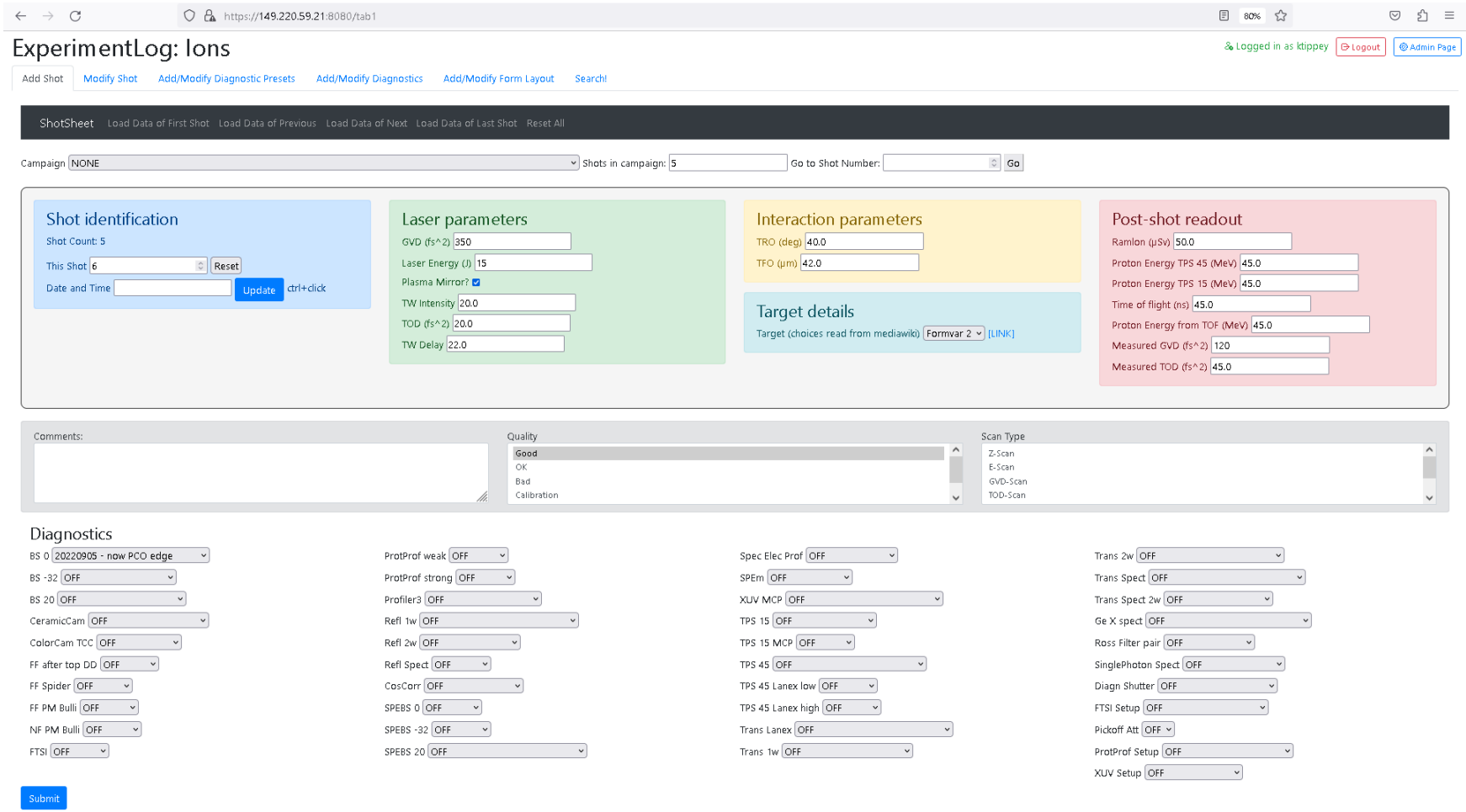
11

Search!

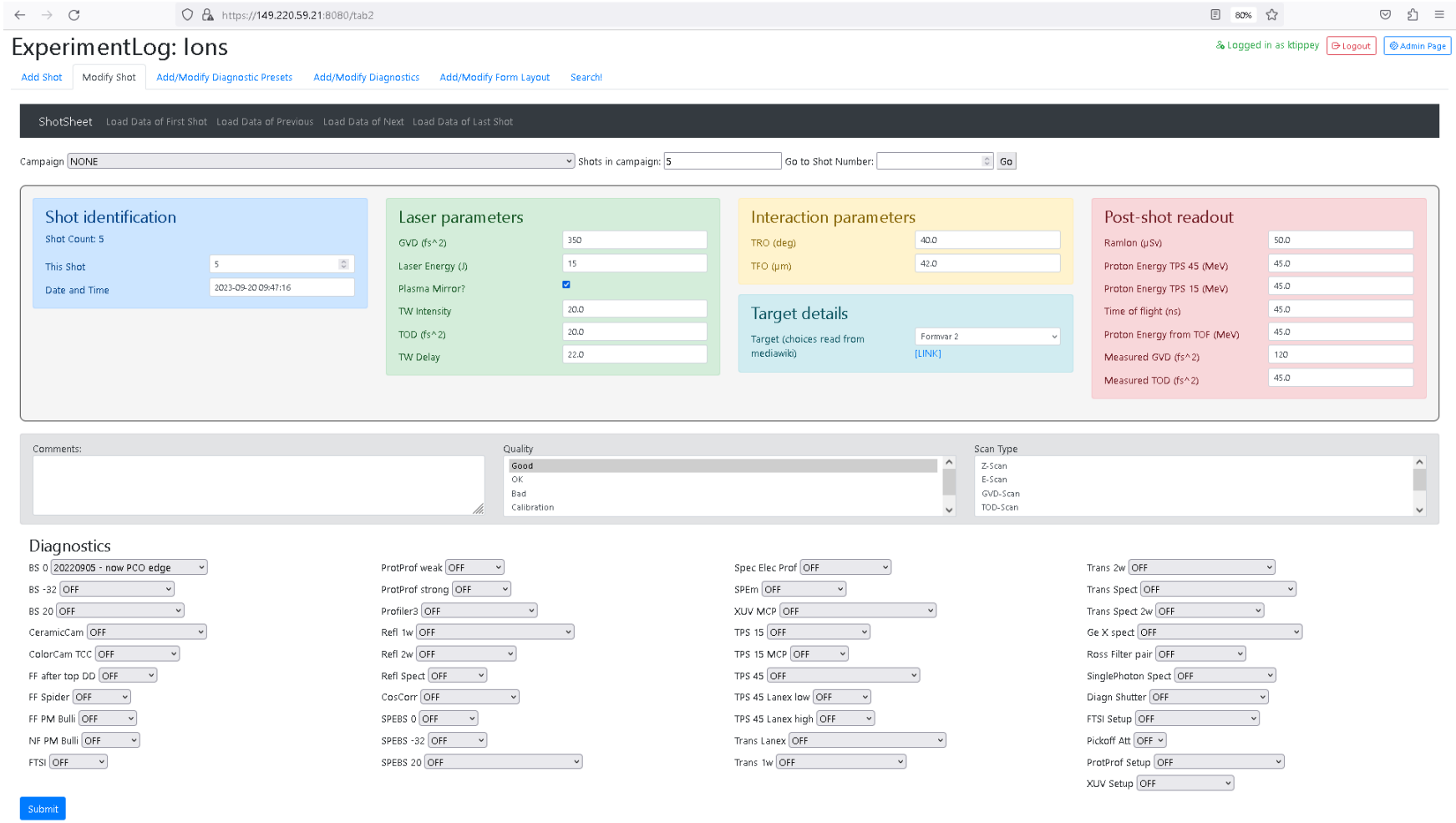


12

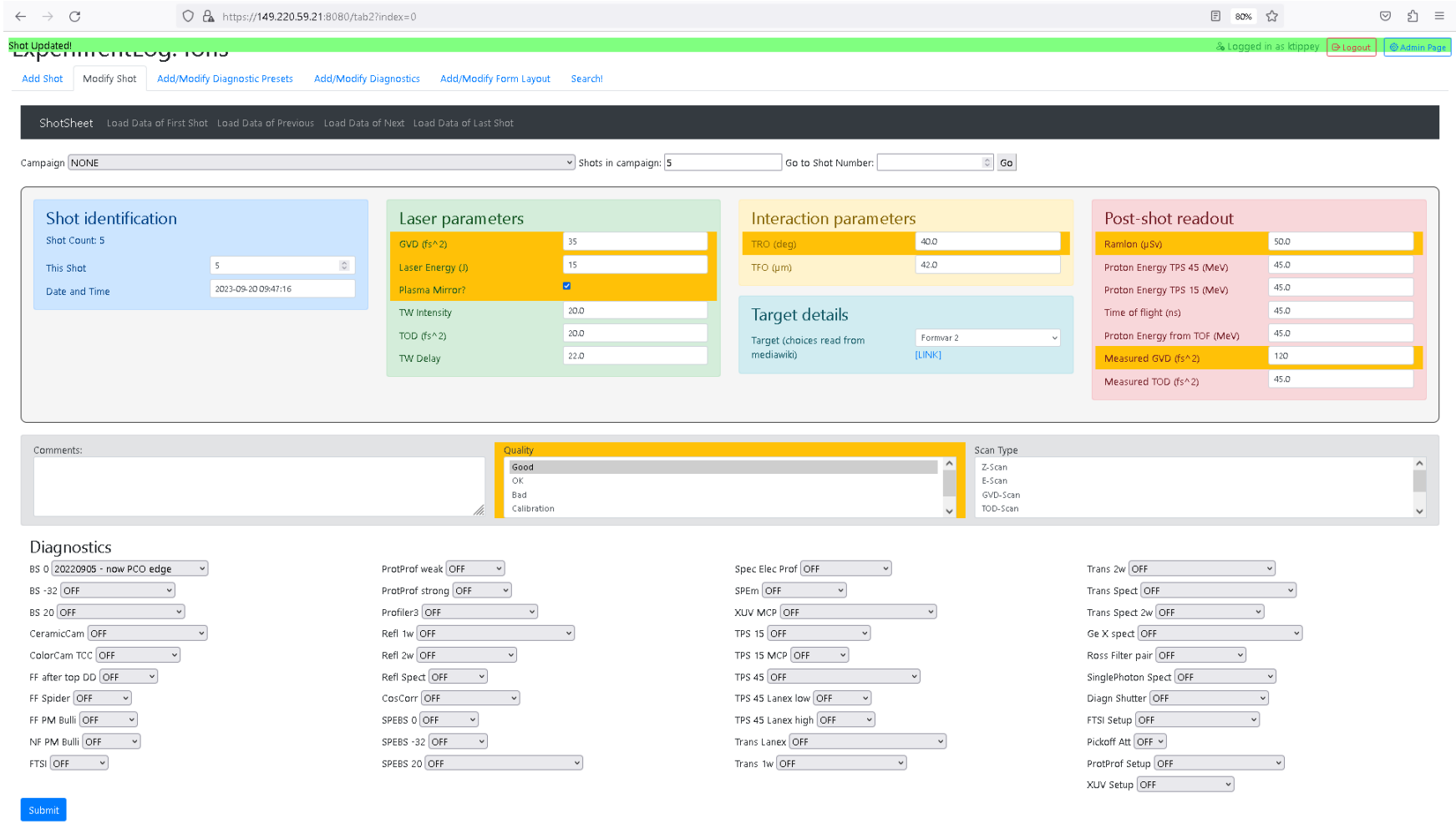
Add Shot


https://149.220.59.21:8080/tab1
ExperimentLog: Ions
Logged in as ktippey
Logout
Admin Page
Add Shot
Modify Shot
Add/Modify Diagnostic Presets
Add/Modify Diagnostics
Add/Modify Form Layout
Search!
ShotSheet
Load Data of First Shot
Load Data of Previous
Load Data of Next
Load Data of Last Shot
Reset All
Campaign NONE
Shots in campaign: 5
Go to Shot Number:
Go
Shot identification
Shot Count: 5
This Shot 6
Reset
Date and Time
Update
ctrl+click
Laser parameters
GVD (fs^2) 350
Laser Energy (J) 15
Plasma Mirror?
TW Intensity 20.0
TOD (fs^2) 20.0
TW Delay 22.0
Interaction parameters
TRO (deg) 40.0
TFO (µm) 42.0
Target details
Target (choices read from mediawiki) Formvar 2
[LINK]
Post-shot readout
Ramlon (µSv) 50.0
Proton Energy TPS 45 (MeV) 45.0
Proton Energy TPS 15 (MeV) 45.0
Time of flight (ns) 45.0
Proton Energy from TOF (MeV) 45.0
Measured GVD (fs^2) 120
Measured TOD (fs^2) 45.0
Comments:
Quality
Good
OK
Bad
Calibration
Scan Type
Z-Scan
E-Scan
GVD-Scan
TOD-Scan
Diagnostics
BS 0 20220905 - now PCO edge
BS -32 OFF
BS 20 OFF
CeramicCam OFF
ColorCam TCC OFF
FF after top DD OFF
FF Spider OFF
FF PM Bulli OFF
NF PM Bulli OFF
FTSI OFF
ProtProf weak OFF
ProtProf strong OFF
Profiler3 OFF
Refl 1w OFF
Refl 2w OFF
Refl Spect OFF
CosCorr OFF
SPEBS 0 OFF
SPEBS -32 OFF
SPEBS 20 OFF
Spec Elec Prof OFF
SPEm OFF
XUV MCP OFF
TPS 15 OFF
TPS 15 MCP OFF
TPS 45 OFF
TPS 45 Lanex low OFF
TPS 45 Lanex high OFF
Trans Lanex OFF
Trans 1w OFF
Trans 2w OFF
Trans Spect OFF
Trans Spect 2w OFF
Ge X spect OFF
Ross Filter pair OFF
SinglePhoton Spect OFF
Diagn Shutter OFF
FTSI Setup OFF
Pickoff Att OFF
ProtProf Setup OFF
XUV Setup OFF
Submit

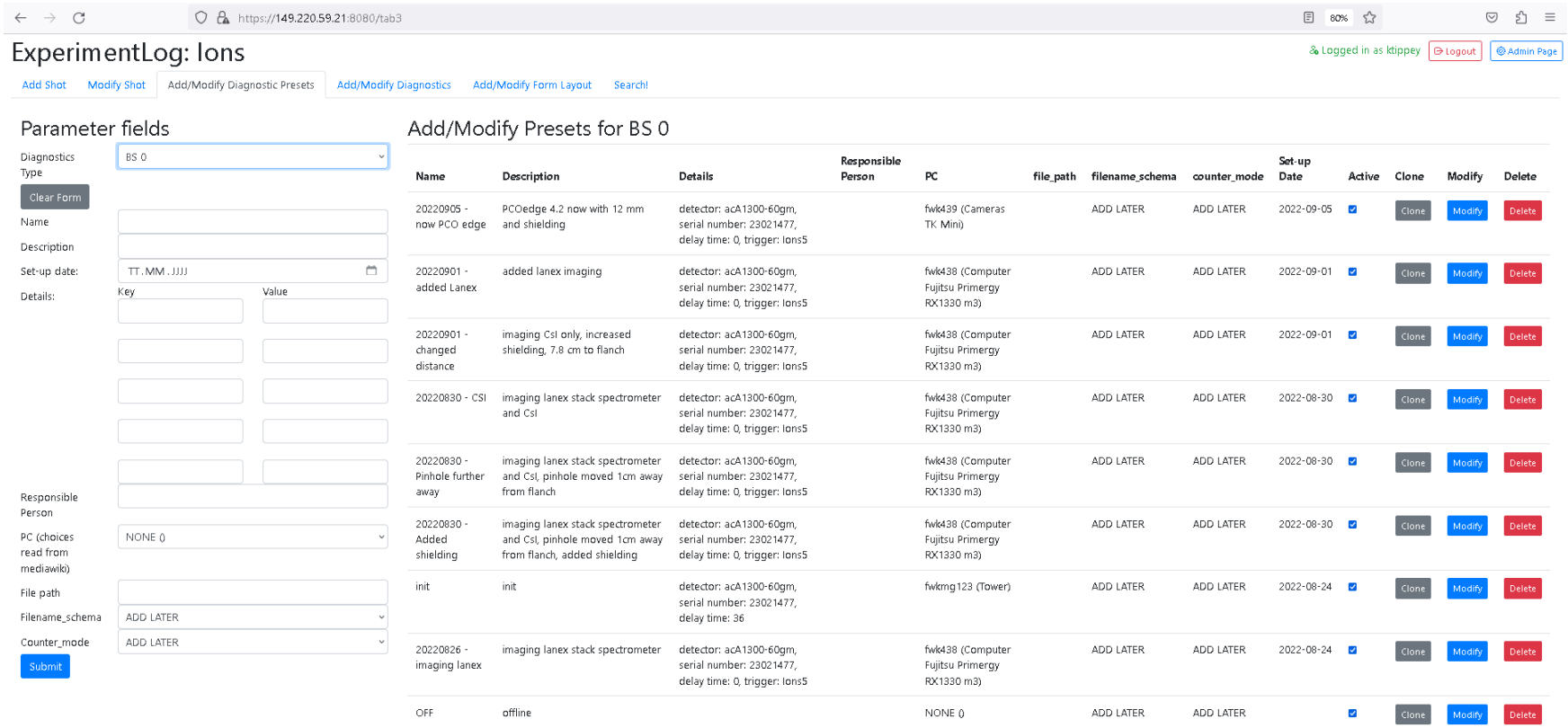
Modify Shot


https://149.220.59.21:8080/tab2
ExperimentLog: Ions
Logged in as ktippey
Logout
Admin Page
Add Shot
Modify Shot
Add/Modify Diagnostic Presets
Add/Modify Diagnostics
Add/Modify Form Layout
Search!
ShotSheet
Load Data of First Shot
Load Data of Previous
Load Data of Next
Load Data of Last Shot
Campaign NONE
Shots in campaign: 5
Go to Shot Number:
Go
Shot identification
Shot Count: 5
This Shot 5
Date and Time 2023-09-20 09:47:16
Laser parameters
GVD (fs^2) 350
Laser Energy (J) 15
Plasma Mirror?
TW Intensity 20.0
TOD (fs^2) 20.0
TW Delay 22.0
Interaction parameters
TRO (deg) 40.0
TFO (µm) 42.0
Target details
Target (choices read from mediawiki) Formvar 2
[LINK]
Post-shot readout
RamIon (µSv) 50.0
Proton Energy TPS 45 (MeV) 45.0
Proton Energy TPS 15 (MeV) 45.0
Time of flight (ns) 45.0
Proton Energy from TOF (MeV) 45.0
Measured GVD (fs^2) 120
Measured TOD (fs^2) 45.0
Comments:
Quality
Good
OK
Bad
Calibration
Scan Type
Z-Scan
E-Scan
GVD-Scan
TOD-Scan
Diagnostics
BS 0 20220905 - now PCO edge
BS -32 OFF
BS 20 OFF
CeramicCam OFF
ColorCam TCC OFF
FF after top DD OFF
FF Spider OFF
FF PM Bulli OFF
NF PM Bulli OFF
FTSI OFF
ProtProf weak OFF
ProtProf strong OFF
Profiler3 OFF
Refl 1w OFF
Refl 2w OFF
Refl Spect OFF
CosCorr OFF
SPEBS 0 OFF
SPEBS -32 OFF
SPEBS 20 OFF
Spec Elec Prof OFF
SPEm OFF
XUV MCP OFF
TPS 15 OFF
TPS 15 MCP OFF
TPS 45 OFF
TPS 45 Lanex low OFF
TPS 45 Lanex high OFF
Trans Lanex OFF
Trans 1w OFF
Trans 2w OFF
Trans Spect OFF
Trans Spect 2w OFF
Ge X spect OFF
Ross Filter pair OFF
SinglePhoton Spect OFF
Diagn Shutter OFF
FTSI Setup OFF
Pickoff Att OFF
ProtProf Setup OFF
XUV Setup OFF
Submit

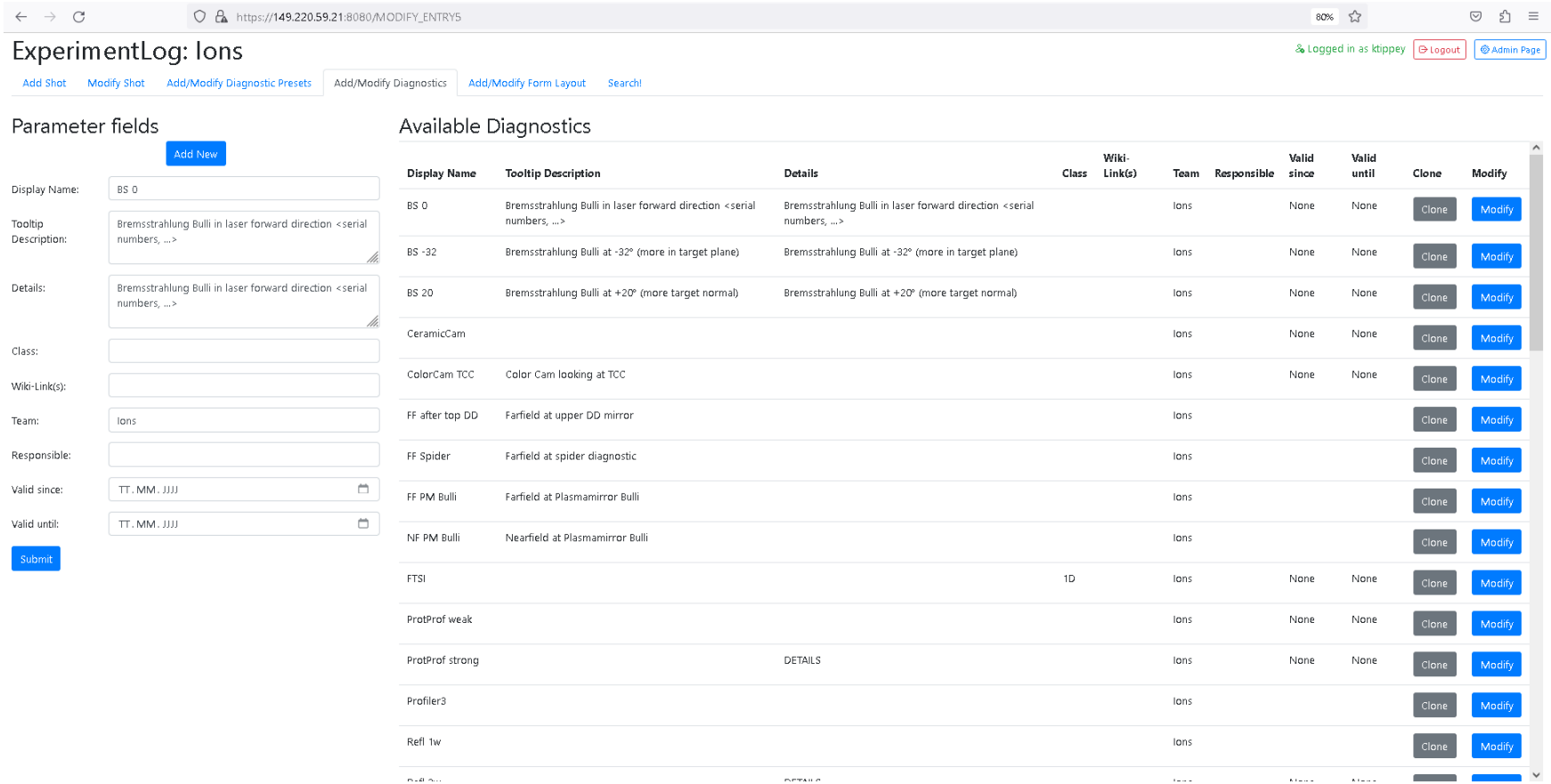
Modify Shot


https://149.220.59.21:8080/tab2?index=0
Shot Updated!
Logged in as ktippey
Logout
Admin Page
Add Shot
Modify Shot
Add/Modify Diagnostic Presets
Add/Modify Diagnostics
Add/Modify Form Layout
Search!
ShotSheet
Load Data of First Shot
Load Data of Previous
Load Data of Next
Load Data of Last Shot
Campaign
NONE
Shots in campaign:
5
Go to Shot Number:
Go
Shot identification
Shot Count: 5
This Shot
5
Date and Time
2023-09-20 09:47:16
Laser parameters
GVD (fs^2)
35
Laser Energy (J)
15
Plasma Mirror?
TW Intensity
20.0
TOD (fs^2)
20.0
TW Delay
22.0
Interaction parameters
TRO (deg)
40.0
TFO (µm)
42.0
Target details
Target (choices read from mediawiki)
Formvar 2
[LINK]
Post-shot readout
Ramion (µSv)
50.0
Proton Energy TPS 45 (MeV)
45.0
Proton Energy TPS 15 (MeV)
45.0
Time of flight (ns)
45.0
Proton Energy from TOF (MeV)
45.0
Measured GVD (fs^2)
120
Measured TOD (fs^2)
45.0
Comments:
Quality
Good
OK
Bad
Calibration
Scan Type
Z-Scan
E-Scan
GVD-Scan
TOD-Scan
Diagnostics
BS 0
20220905 - now PCO edge
BS -32
OFF
BS 20
OFF
CeramicCam
OFF
ColorCam TCC
OFF
FF after top DD
OFF
FF Spider
OFF
FF PM Bulli
OFF
NF PM Bulli
OFF
FTSI
OFF
ProtProf weak
OFF
ProtProf strong
OFF
Profiler3
OFF
Refl 1w
OFF
Refl 2w
OFF
Refl Spect
OFF
CosCorr
OFF
SPEBS 0
OFF
SPEBS -32
OFF
SPEBS 20
OFF
Spec Elec Prof
OFF
SPEm
OFF
XUV MCP
OFF
TPS 15
OFF
TPS 15 MCP
OFF
TPS 45
OFF
TPS 45 Lanex low
OFF
TPS 45 Lanex high
OFF
Trans Lanex
OFF
Trans 1w
OFF
Trans 2w
OFF
Trans Spect
OFF
Trans Spect 2w
OFF
Ge X spect
OFF
Ross Filter pair
OFF
SinglePhoton Spect
OFF
Diagn Shutter
OFF
FTSI Setup
OFF
Pickoff Att
OFF
ProtProf Setup
OFF
XUV Setup
OFF
Submit

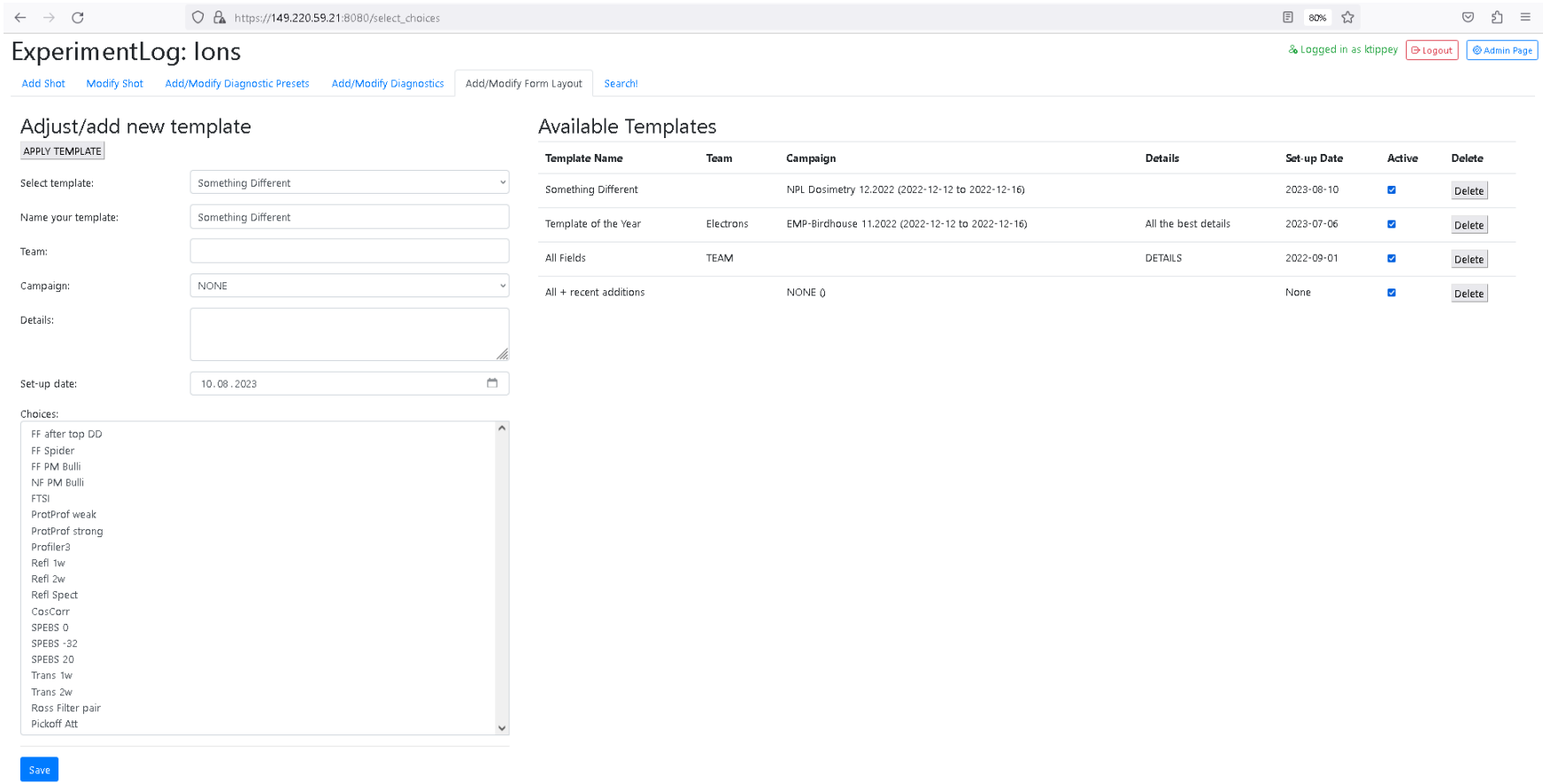
Add/Modify Diagnostic Presets



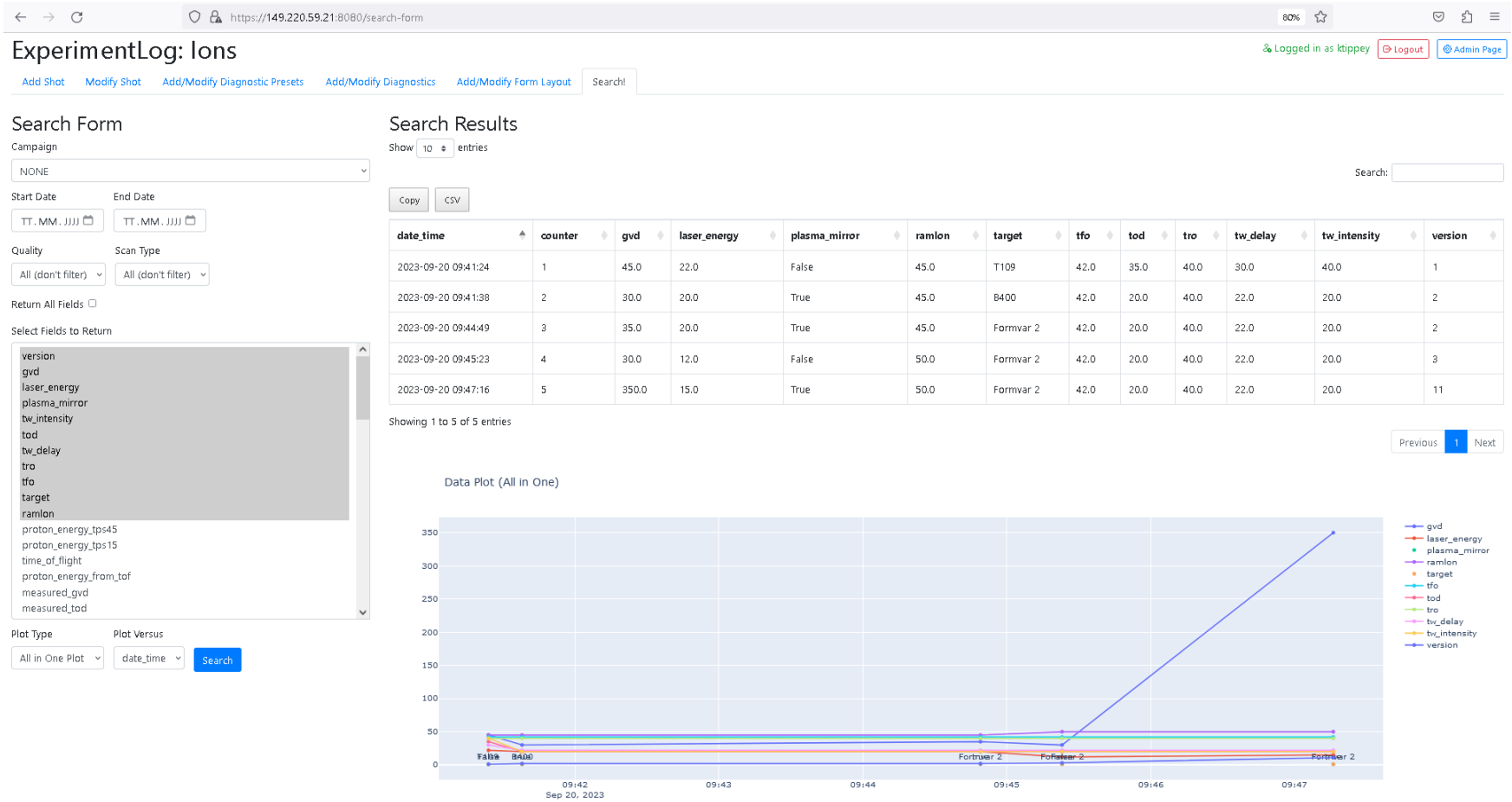
Add/Modify Diagnostics



Add/Modify Form Layout

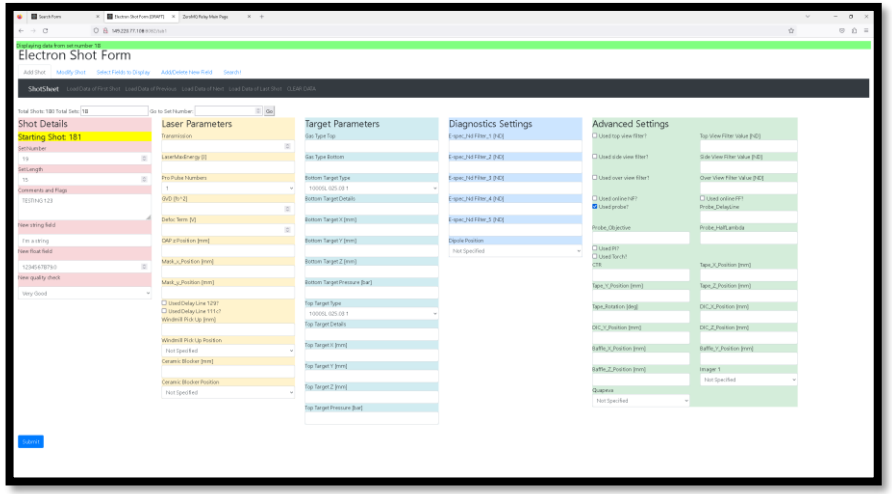


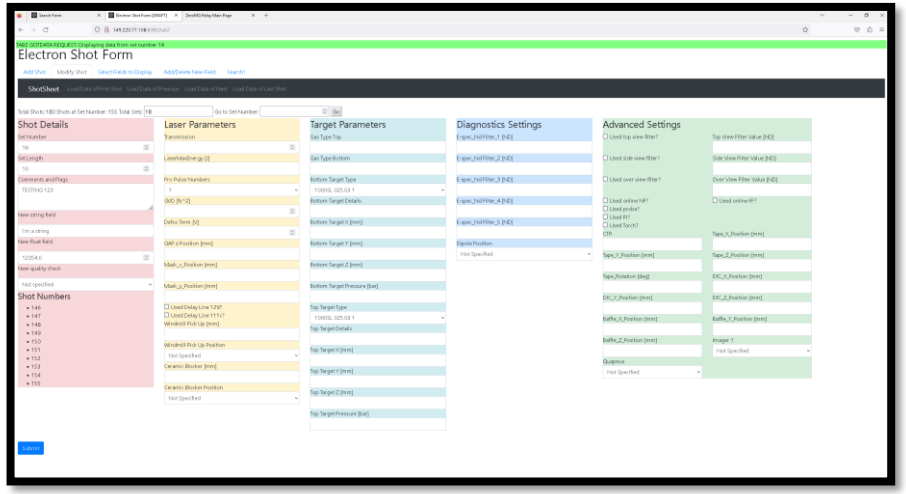
Search!

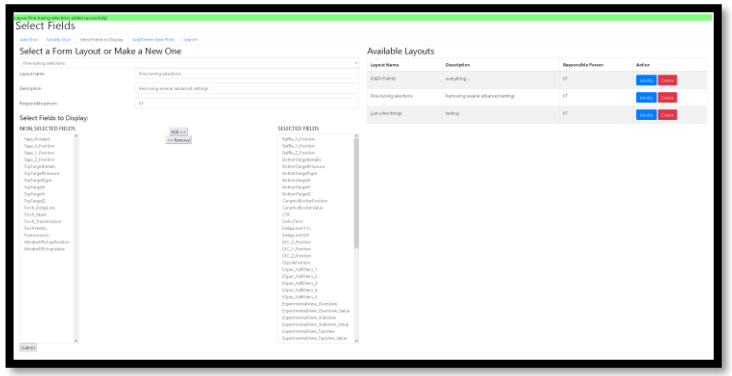

https://149.220.59.21:8080/search-form
ExperimentLog: Ions
Logged in as ktippey
Logout
Admin Page
Add Shot
Modify Shot
Add/Modify Diagnostic Presets
Add/Modify Diagnostics
Add/Modify Form Layout
Search!
Search Form
Campaign
NONE
Start Date
End Date
TT . MM . JJJJ
Quality
Scan Type
All (don't filter)
Return All Fields
Select Fields to Return
version
gvd
laser_energy
plasma_mirror
tw_intensity
tod
tw_delay
tro
tfo
target
ramlon
proton_energy_tps45
proton_energy_tps15
time_of_flight
proton_energy_from_tof
measured_gvd
measured_tod
Plot Type
All in One Plot
Plot Versus
date_time
Search
Search Results
Show 10 entries
Search:
Copy
CSV
date_time
counter
gvd
laser_energy
plasma_mirror
ramlon
target
tfo
tod
tro
tw_delay
tw_intensity
version
2023-09-20 09:41:24 1 45.0 22.0 False 45.0 T109 42.0 35.0 40.0 30.0 40.0 1
2023-09-20 09:41:38 2 30.0 20.0 True 45.0 B400 42.0 20.0 40.0 22.0 20.0 2
2023-09-20 09:44:49 3 35.0 20.0 True 45.0 Formvar 2 42.0 20.0 40.0 22.0 20.0 2
2023-09-20 09:45:23 4 30.0 12.0 False 50.0 Formvar 2 42.0 20.0 40.0 22.0 20.0 3
2023-09-20 09:47:16 5 350.0 15.0 True 50.0 Formvar 2 42.0 20.0 40.0 22.0 20.0 11
Showing 1 to 5 of 5 entries
Previous
1
Next
Data Plot (All in One)
350
300
250
200
150
100
50
0
09:42
Sep 20, 2023
09:43
09:44
09:45
09:46
09:47
gvd
laser_energy
plasma_mirror
ramlon
target
tfo
tod
tro
tw_delay
tw_intensity
version

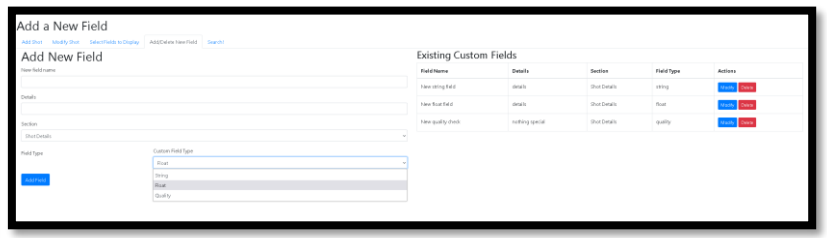
Shotsheet [electrons]: The different tabs

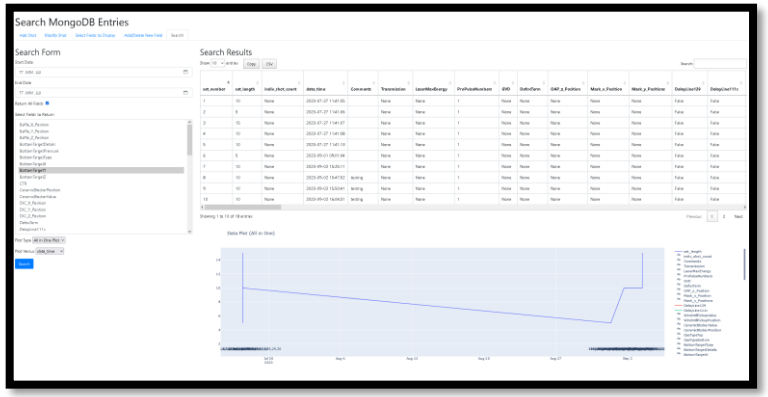
Outline





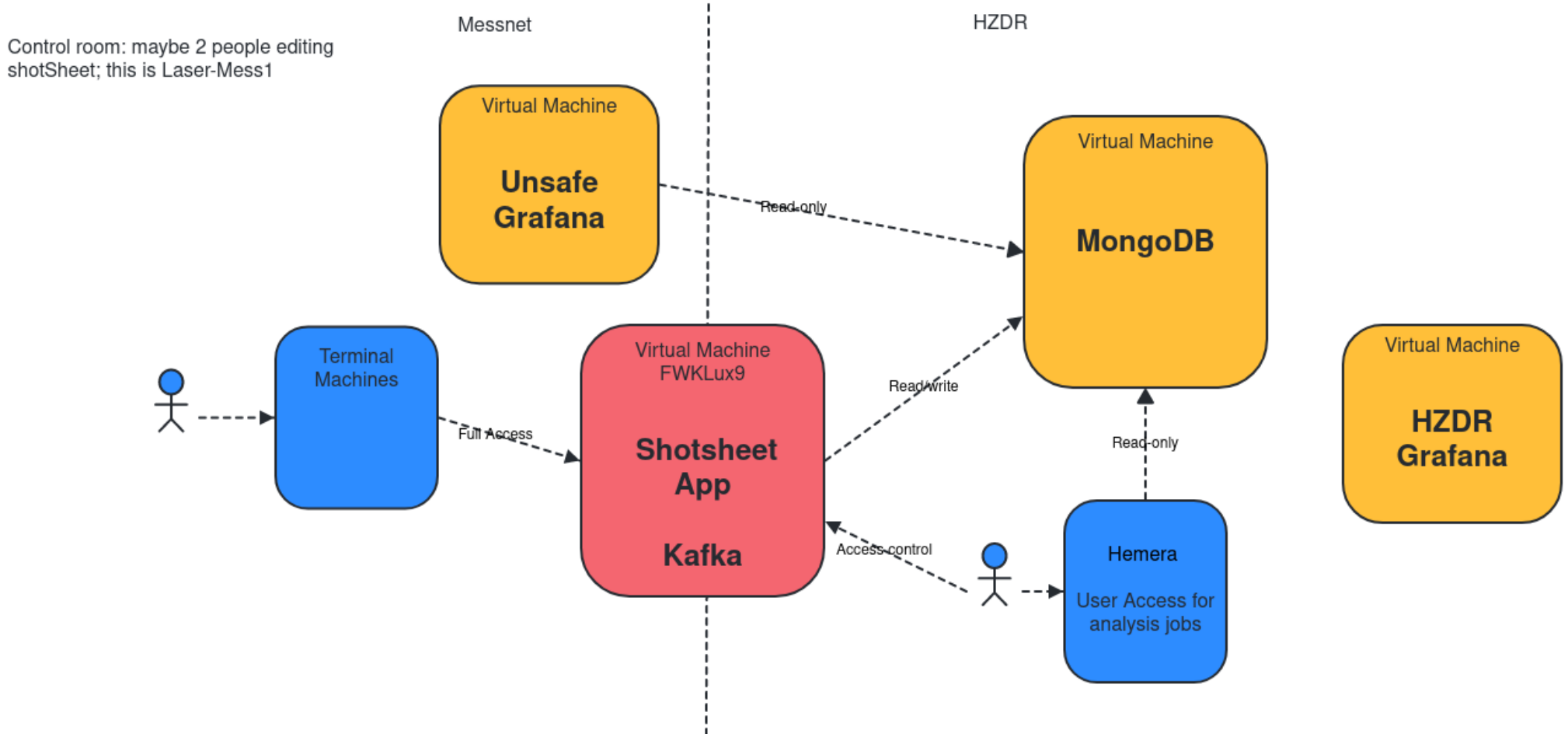






Shotsheet: Basic Setup

Planned deployment implementation



Demo?

Check out our WIKI page – https://athene.fz-rossendorf.de/fwk/FWKT:ShotSheet_(ExL)

IONS*

https://149.220.59.21:8080/

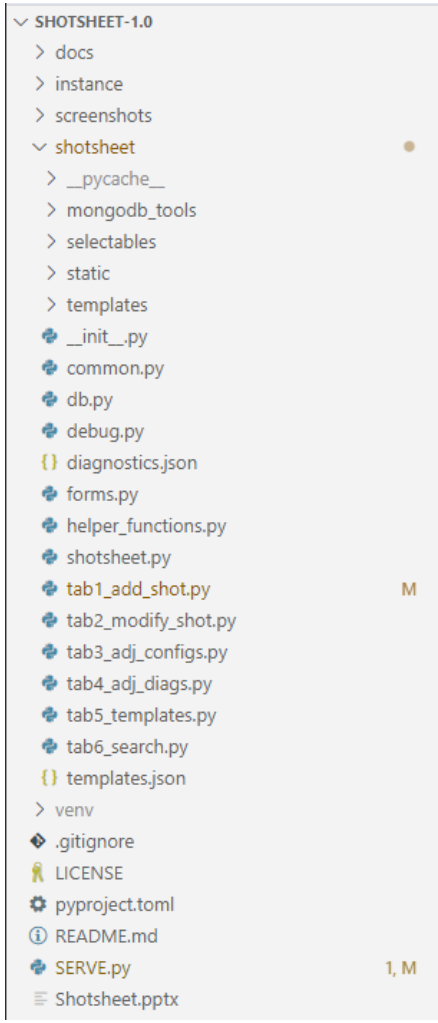
ELECTRONS*

https://149.220.59.21:8082/

* HTTPS for security and to alleviate CSRF token errors from when using regular http

* Currently self-certified https, working on getting real certificates and memorable server names on fwklux9/m:

- https://shotsheet-ions.fz-rossendorf.de:8080
- https://shotsheet-electrons.fz-rossendorf.de:8082
- https://kafkawatcher.fz-rossendorf.de:9999



ZeroMQ Relay: LabView vs. Flask for Draco Shot Counter

FWK573

Labview ZeroMQ Relay

No ability to message out with Kafka

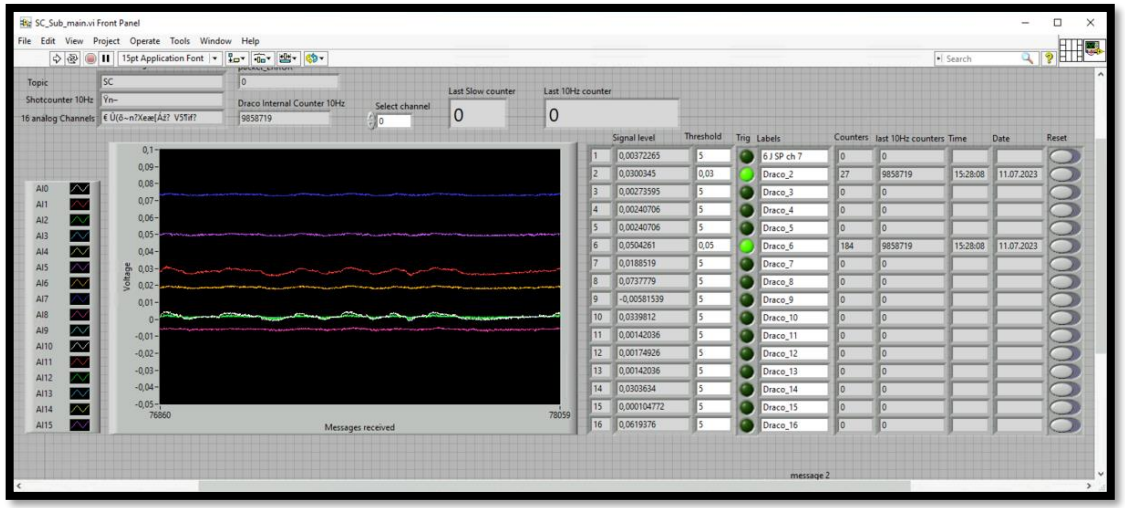
Complicated license situation

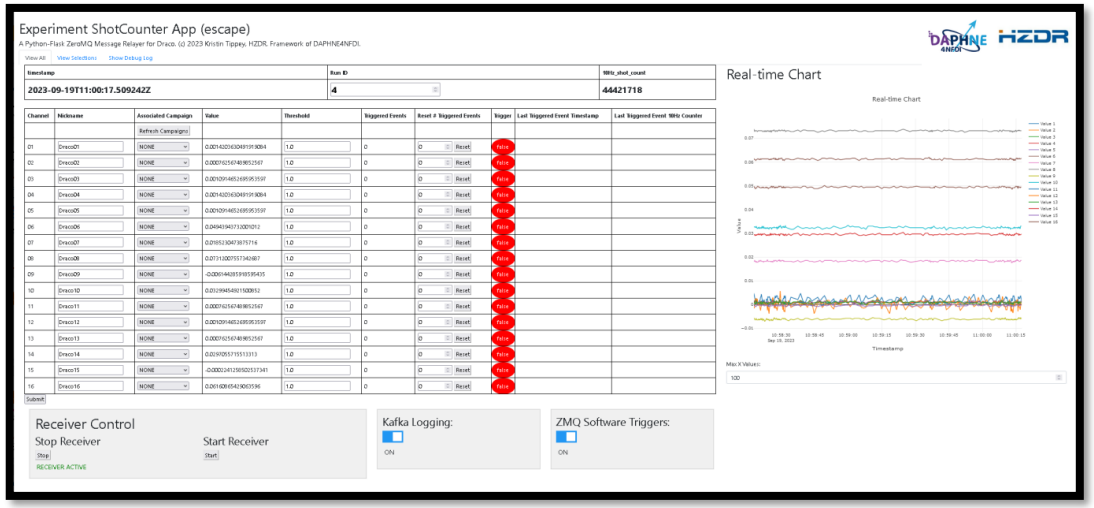
->

Python Flask ZeroMQ Relay

Able to message directly out with Kafka

No license issues

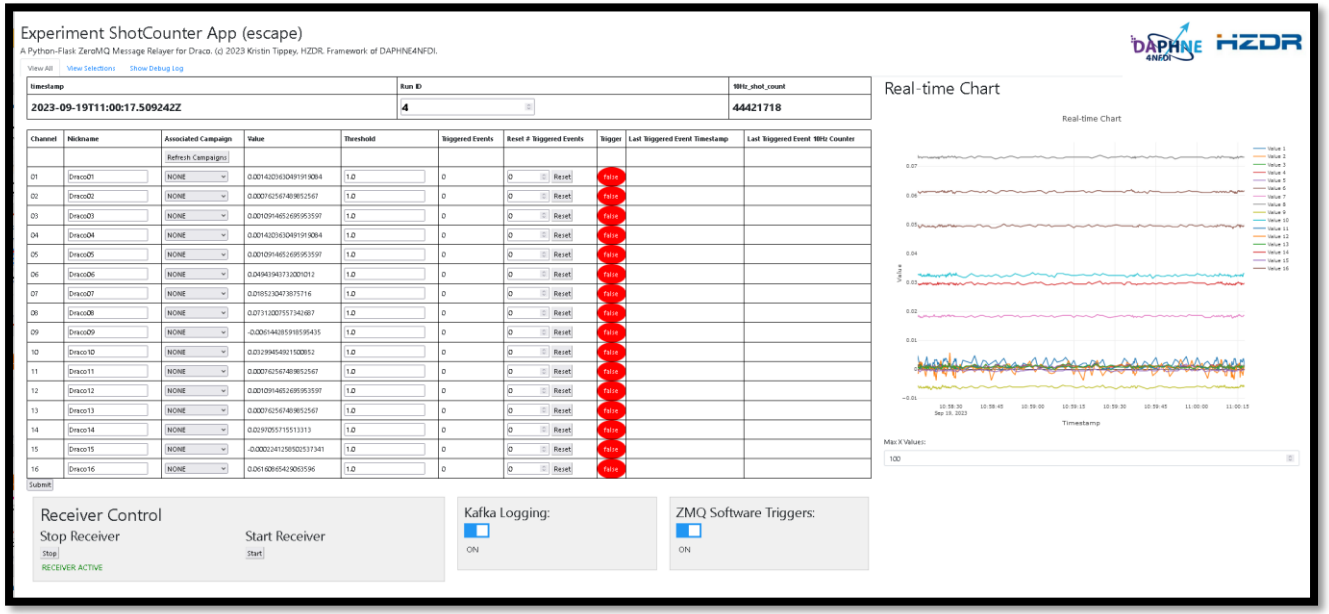




LabView Credit: Wolfgang Horn

python waitress-serve --port=8888 zeromq_relay:app

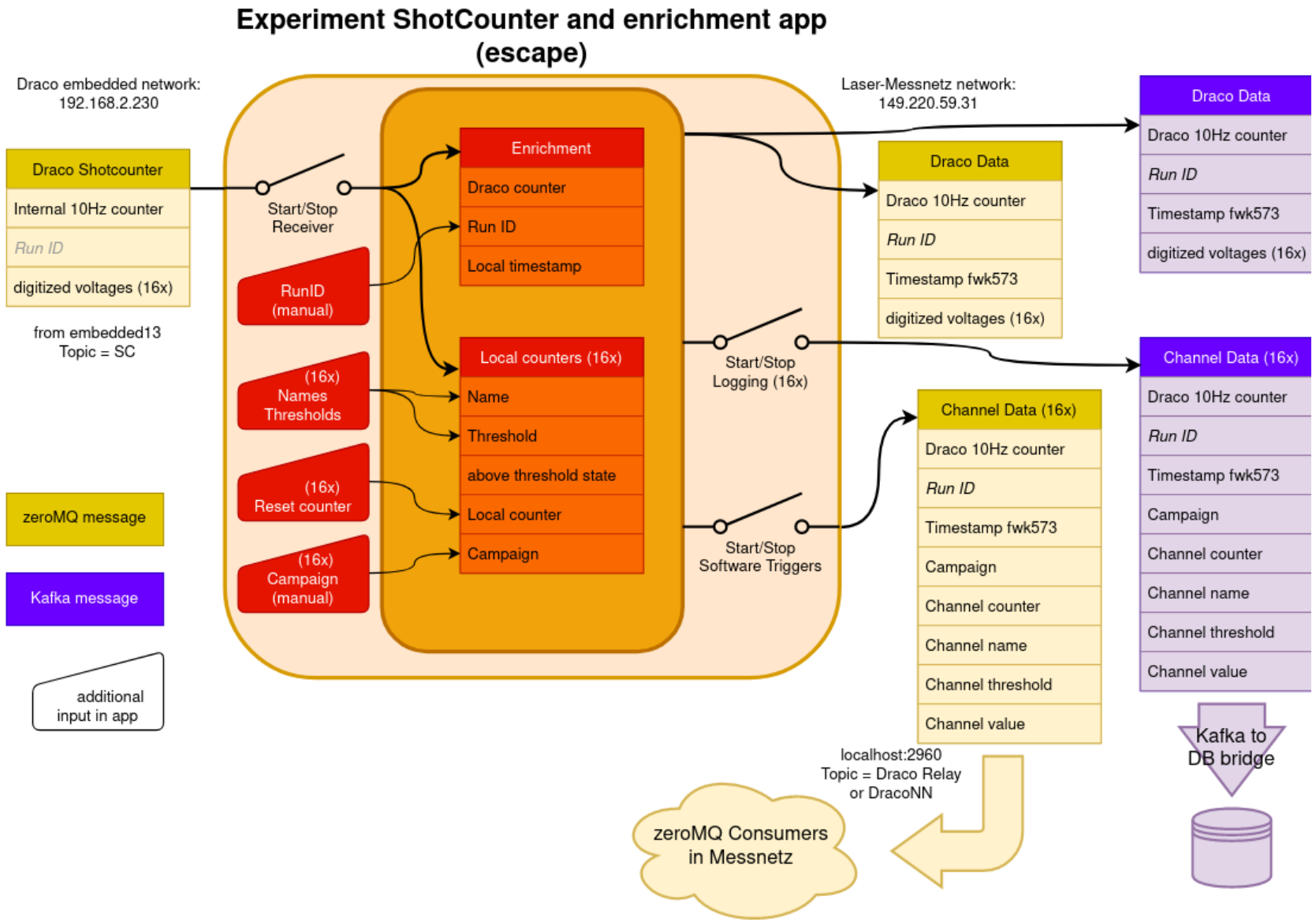
ZeroMQ Relay: Main page, selection page, debug page

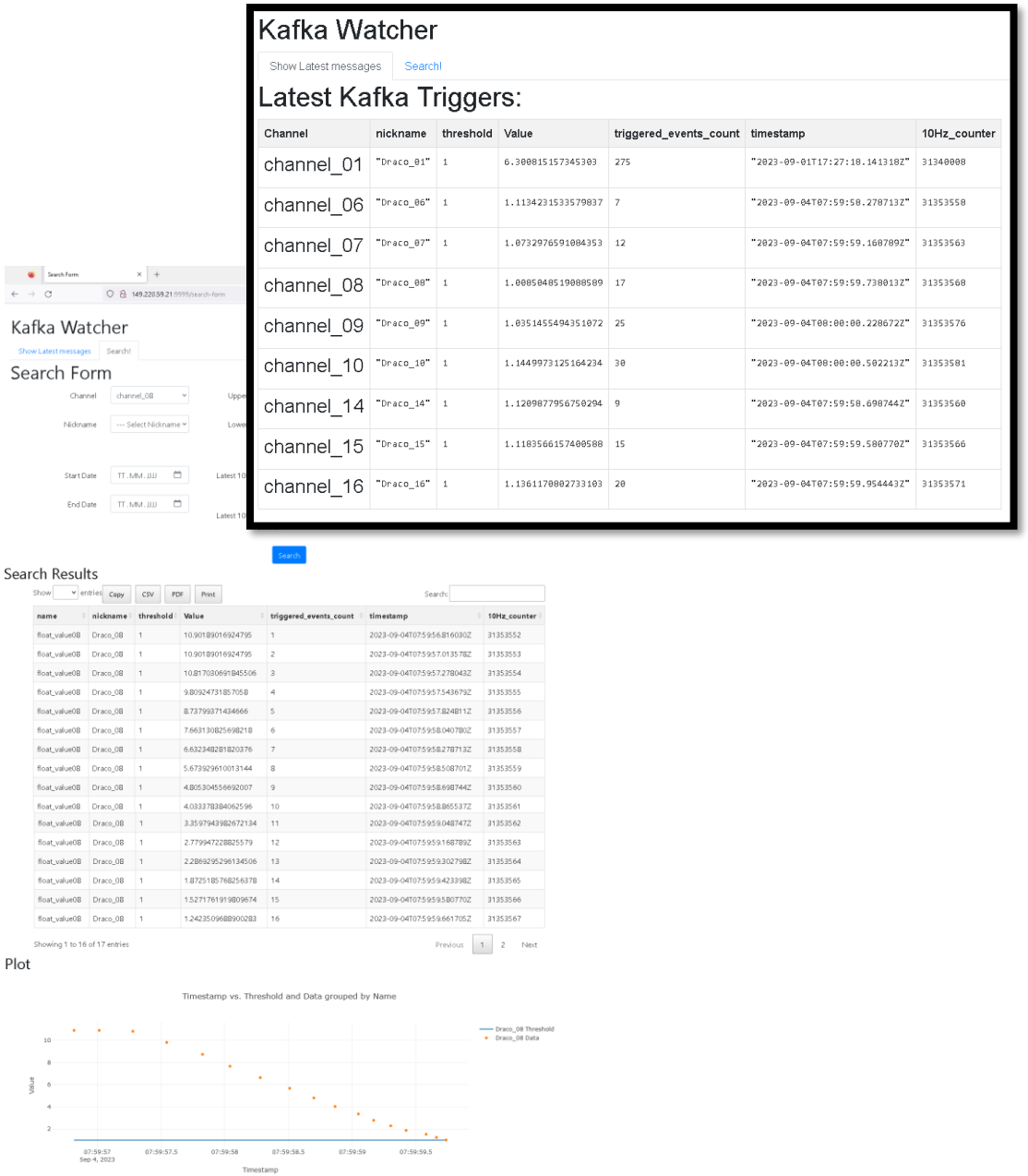


- Displays incoming ZeroMQ data in tabular and graphical form
- User input of nicknames, campaigns, thresholds, local trigger counts
- Triggers upon incoming values > threshold values
- Relays ***triggered data*** to Kafka (MongoDB) and ***all data*** to ZeroMQ (future: software triggers)

Demo?

http://149.220.59.31:8888/


Experiment ShotCounter and enrichment app
(escape)
Draco embedded network:
192.168.2.230
Draco Shotcounter
Internal 10Hz counter
Run ID
digitized voltages (16x)
from embedded13
Topic = SC
Start/Stop
Receiver
RunID
(manual)
(16x)
Names
Thresholds
(16x)
Reset counter
(16x)
Campaign
(manual)
Enrichment
Draco counter
Run ID
Local timestamp
Local counters (16x)
Name
Threshold
above threshold state
Local counter
Campaign
Laser-Messnetz network:
149.220.59.31
Start/Stop
Logging (16x)
Start/Stop
Software Triggers
Draco Data
Draco 10Hz counter
Run ID
Timestamp fwk573
digitized voltages (16x)
Channel Data (16x)
Draco 10Hz counter
Run ID
Timestamp fwk573
Campaign
Channel counter
Channel name
Channel threshold
Channel value
Draco Data
Draco 10Hz counter
Run ID
Timestamp fwk573
digitized voltages (16x)
Channel Data (16x)
Draco 10Hz counter
Run ID
Timestamp fwk573
Campaign
Channel counter
Channel name
Channel threshold
Channel value
Kafka to
DB bridge
localhost:2960
Topic = Draco Relay
or DracoNN
zeroMQ Consumers
in Messnetz
zeroMQ message
Kafka message
additional
input in app



Kafka Receiver and Relay to MongoDB

- Shows incoming Kafka messages in real time, relays them to MongoDB, and allows you to search through all the entries

Specifics:

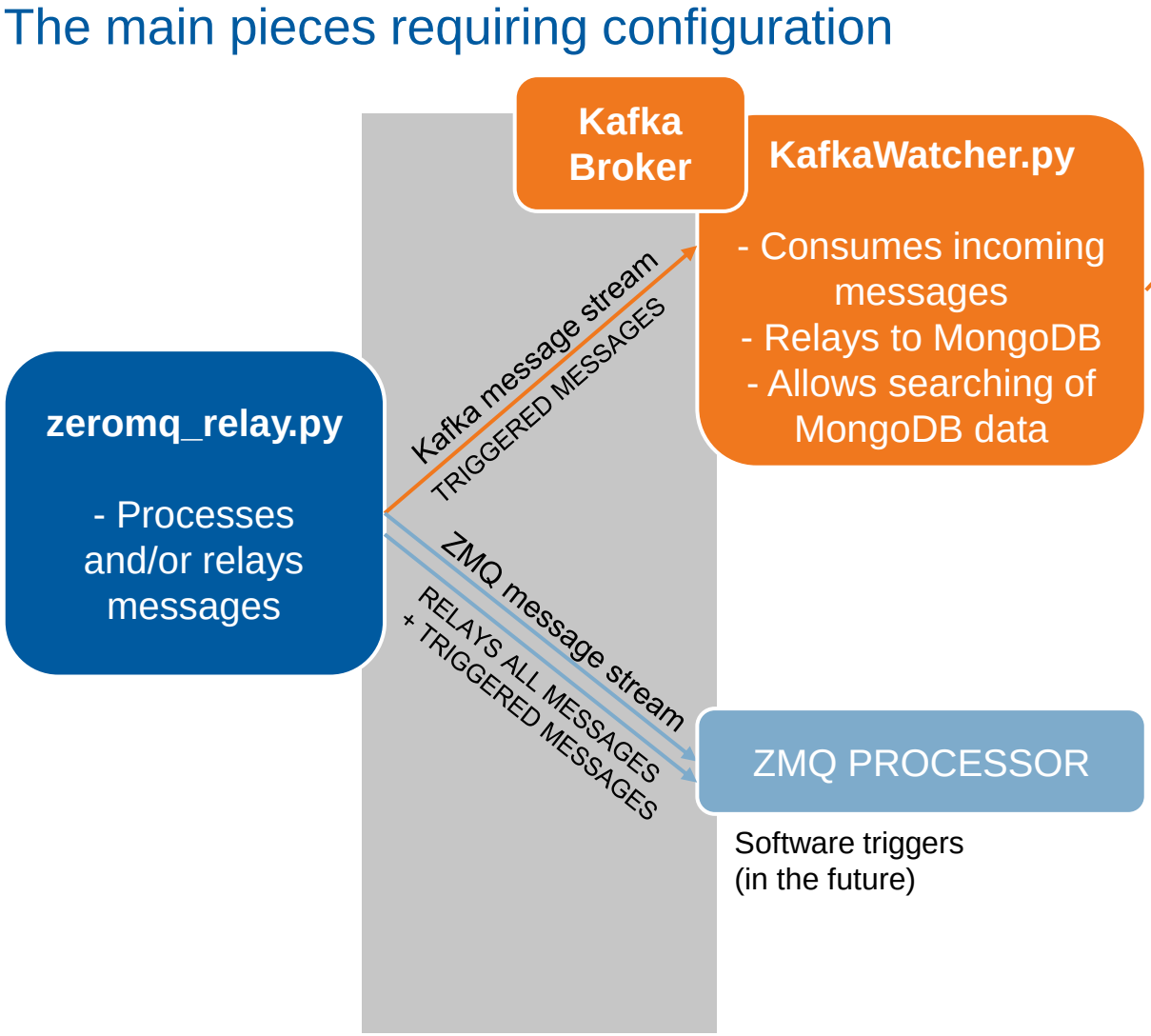
- Connected to kafka broker on fwklux9
- Serve KafkaWatcher from fwklux9 with:

  gunicorn --certfile=cert.pem --keyfile=key.pem --worker-class eventlet -w 1 -b 0.0.0.0:9999 "KafkaGUI:create_app()"

- Access on FWKTS07 or another computer on the network at https://149.220.59.21:9999/

ZeroMQ Relay and KafkaWatcher: Basic Setup

The main pieces requiring configuration

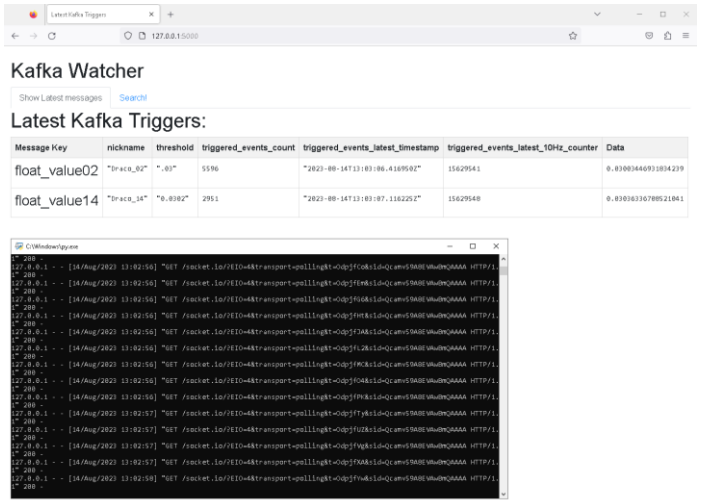


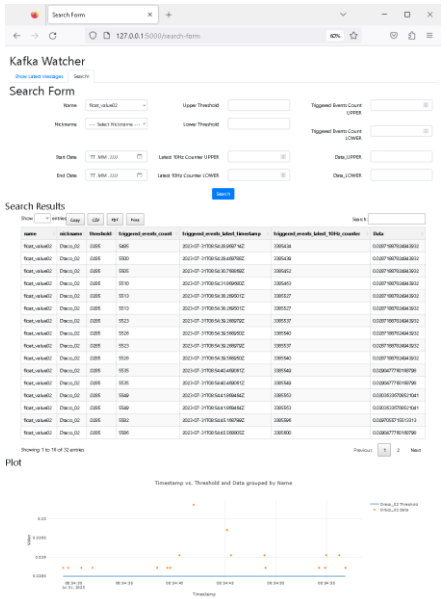
MongoDB

Currently only limited test data

KT_mongoDB_GUI.py

- Allows searching of MongoDB data





ZeroMQ Relay and KafkaGUI: Where to get the different pieces

zeromq_relay.py

- Processes and/or relays messages

…/zeromq-broker

Kafka Broker

KafkaWatcher.py

- Consumes incoming messages
- Relays to MongoDB
- Allows searching of MongoDB data

…/kafka-gui

…/fwklux9-kafka

MongoDB

Currently only limited test data

> Generated test read-only account

> Working on getting new db specifically for this purpose

KT_mongoDB_GUI.py

- Allows searching of MongoDB data

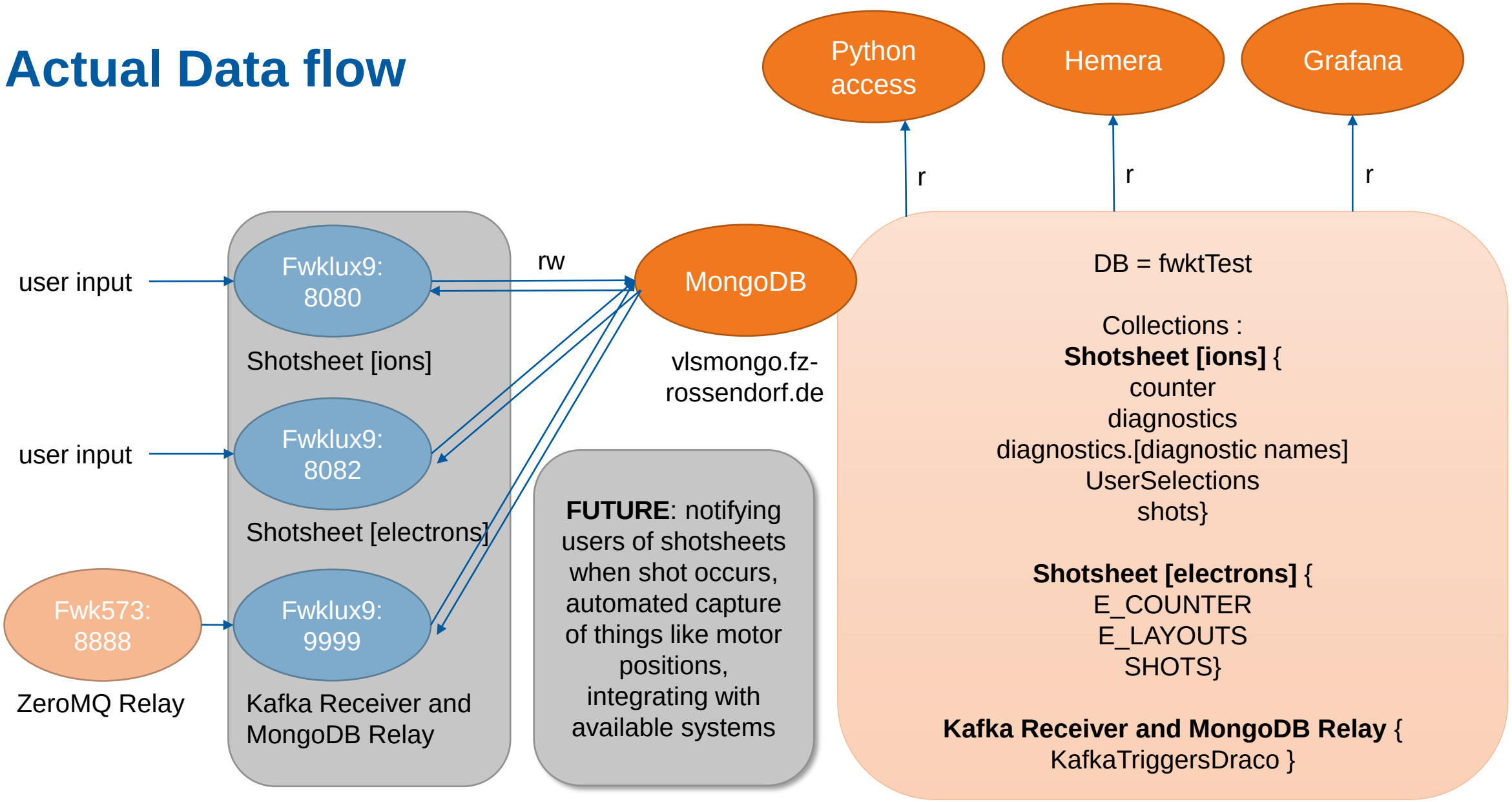
…/kafka-triggers-mongodb-gui

> Can be run from anywhere you can access the MongoDB

Hosted by GitLab

Still under development but available upon request.
Plan to share publicly.

Actual Data flow



Add-On: SciCat Upload Tools for Simulationists

Developed SciCat metadata extraction and upload to SciCat tools for

- Smilei: extracts input.py files
- picmi-PIConGPU: extracts from python files
- PIConGPU: extracts from cfg, param files across folders. Working on improved extraction mechanisms, curation
- WarpX: extracts from txt input file

Currently undergoing testing and refinement

Configuring beyond scripts into GUI's? Flask?

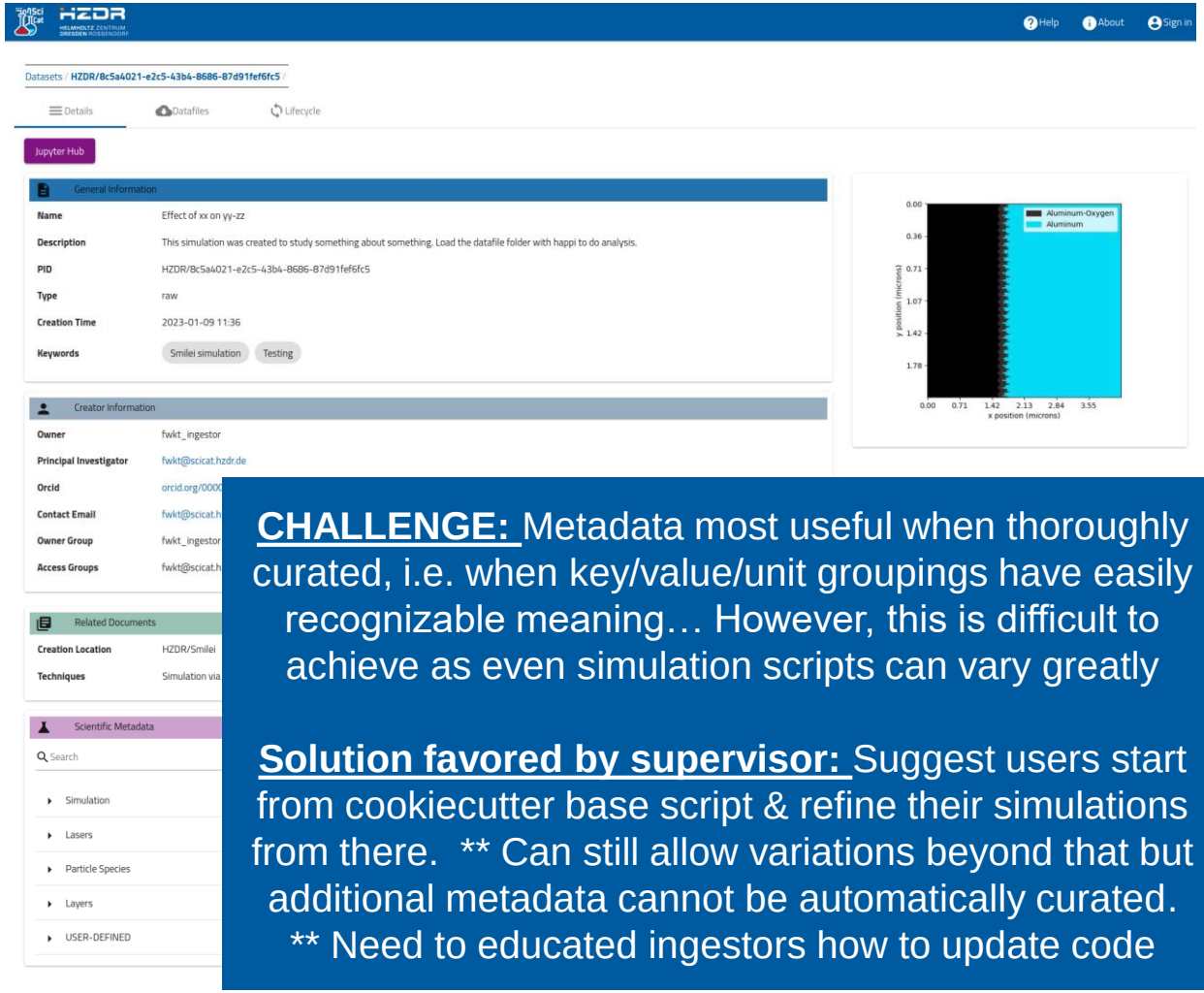
Smilei

PIConGPU

ECP-WarpX/**WarpX**

WarpX is an advanced, time-based electromagnetic & electrostatic Particle-In-Cell code.

77 Contributors · 280 Issues · 13 Discussions · 203 Stars · 142 Forks



CHALLENGE: Metadata most useful when thoroughly curated, i.e. when key/value/unit groupings have easily recognizable meaning… However, this is difficult to achieve as even simulation scripts can vary greatly

Solution favored by supervisor: Suggest users start from cookiecutter base script & refine their simulations from there. ** Can still allow variations beyond that but additional metadata cannot be automatically curated. ** Need to educated ingestors how to update code

Review

Current: Developed apps for research data management application, focus around improving shot tracking

- Shotsheet: Currently entirely manual data logging (served with gunicorn by fwklux9)
- ZeroMQ Relay: Tracks and relays shot triggers sent from Draco laser (served with waitress by fwk573 gateway) via KafkaBroker (hosted by fwklux9)
- Kafka Receiver and MongoDB Relay: Receives real-time kafka messages from KafkaBroker and emits to WebApp for monitoring, sends to mongoDB for logging and searching (served with gunicorn by fwklux9)

Additionally, for simulations, uploader tools allow uploading of curated metadata to SciCat

Future: Integrate with existing systems, mediawiki, motor trackers, etc. towards automation, integrate directly with SciCat, …

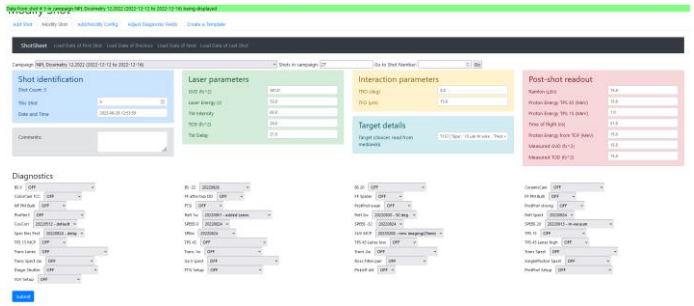
** We hope to improve on these apps and work further with experimentalists and simulationists towards an increasingly streamlined data/metadata pipeline **

Thank you for your attention

Questions? Suggestions? Collaboration ideas?

Hosted by: Fwklux9:8080, 8082

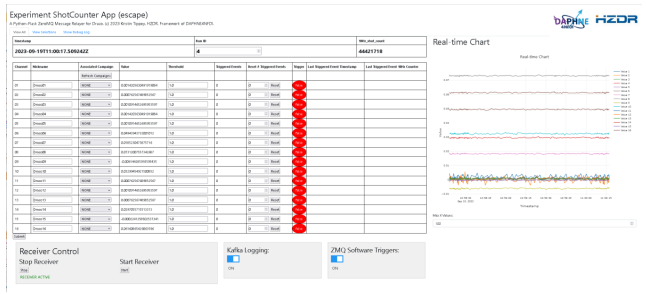
Shotsheet [ions] and [electrons] https://149.220.59.21:8080/ https://149.220.59.21:8082/



Fwk573:8888

ZeroMQ Relay

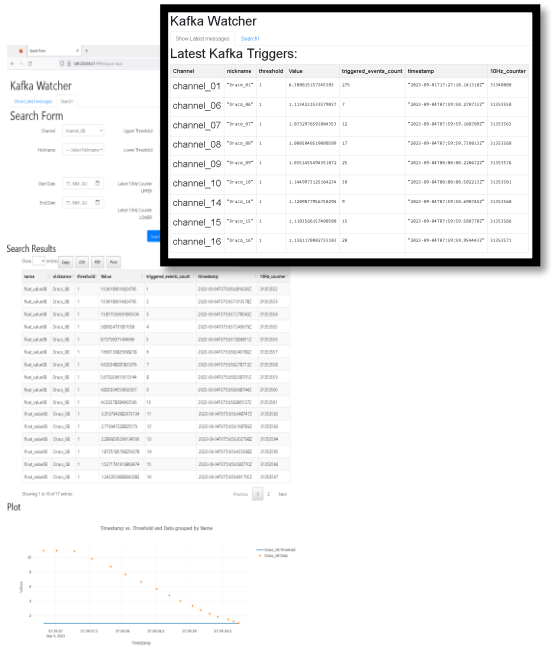
http://149.220.59.31:8888/



Fwklux9:9999

Kafka Receiver and MongoDB Relay

https://149.220.59.21:9999/



SciCat Upload Tools

k.tippey@hzdr.de