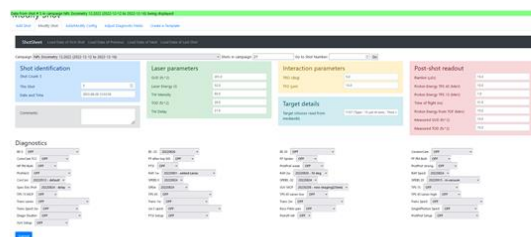


Hosted by:

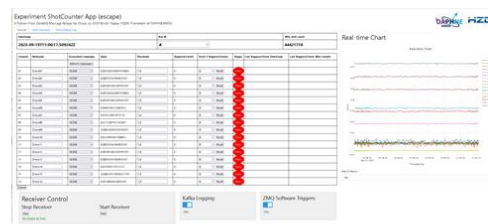
Fwklux9:8080,
8082

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



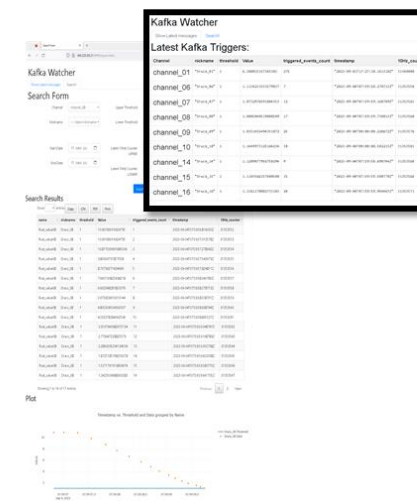
Fwk573:8888

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

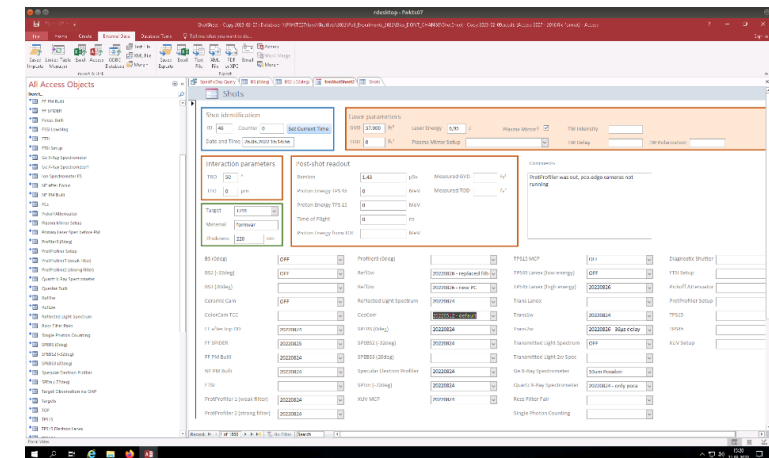
Started as Excel

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

[illegible]

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 microframework with wide range of supported features
--------------	--

MongoDB NoSQL document-based database

Other supporting Elements

WTForms form validation

Javascript dynamic features

Jinja2

Bootstrap clean consistent form layouts

Shot ID

Modify Shot

AddModfly Settings

AddModfly Diagnostics

AddModfly 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: MPFL_Sets 2023 (2023-09-04 to 2023-09-11)

Go to Shot Number:

Go

Shot identification

Shot Count: 0

This Shot: 1

Reset

Date and Time: 2023-09-25 09:04:12

Submit

add-link

Laser parameters

GVD [ps²]: 20.0

Laser Energy [J]: 15.0

Pulse Minus? ☐

FW intensity: 20.0

TOD [ps²]:

TW Delay:

Interaction parameters

TRO [ps]:

TFO [ps]:

Target details

Target (choices read from mediawiki)

TSP (Type: "30 psi Water", Thickness: "15 psi")

Post-shot readout

Random [g/s]: 50.0

Proton Energy TPS 45 (MeV):

Proton Energy TPS 15 (MeV):

Time of Flight [ns]:

Proton Energy from TDF (GeV):

Measured GVD [ps²]:

Measured TOD [ps³]:

Comments:

Quality

Good

OK

Bad

Calibration

Scan Type

2-Scan

6-Scan

GVD-Scan

TOD-Scan

Diagnostics

BS 0 QOFF

ColorCam TCC QOFF

RF PM Bulk QOFF

Proton QOFF

CrucCam QOFF

Spec Elec Prof QOFF

TPS 15 MCP QOFF

Trans Lanes QOFF

Trans Speed 2w QOFF

Diagn Shutter QOFF

XUV Setup QOFF

BS 32 QOFF

FF after top dog QOFF

FTIS QOFF

Red 1w QOFF

SPERS 0 QOFF

SPERN QOFF

TPS 45 QOFF

Trans 3w QOFF

Gas X Spot QOFF

FTIS Setup QOFF

BS 20 QOFF

FF Spider QOFF

ProthProf read QOFF

Red 2w QOFF

SPERS 2w QOFF

XUV MCP QOFF

TPS 45 Lanes Low QOFF

Trans 2w QOFF

Rock Filter pos QOFF

Pickoff Ad QOFF

GenCamCam QOFF

FF PM Bulk QOFF

ProthProf strong QOFF

Red Specs QOFF

SPERS 2w QOFF

TPS 15 QOFF

TPS 45 Lanes High QOFF

Trans Specs QOFF

SinglePhoton Specs QOFF

ProthProf Setup QOFF

Search MongoDB Entries

not used

modify data

AddModfly Settings

AddModfly Diagnostics

AddModfly Form Layout

Search

Search Form

Search Results

Graph

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

← → ↻ https://149.220.59.21:8080/login 80% ☆

ExperimentLog: Ions [Login](#)

[Add Shot](#) [Modify Shot](#) [Add/Modify Diagnostic Presets](#) [Add/Modify Diagnostics](#) [Add/Modify Form Layout](#) [Search!](#)

Username

Role

[Login](#)

← → ↻ https://149.220.59.21:8080/admin 80% ☆

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!](#)

Currently Logged-in Users:

Username	Role	IP Address	Action
ktippey	admin	149.220.58.248	

Shotsheet [ions]: The different tabs

Outline

Add Shot

11.10.2023 Advancing Research Data Management with Python-Flask Applications



7

Modify Shot

11.10.2023 Advancing Research Data Management with Python-Flask Applications



8

Add/Modify Diagnostic Presets

11.10.2023 Advancing Research Data Management with Python-Flask Applications



9

Add/Modify Diagnostics

11.10.2023 Advancing Research Data Management with Python-Flask Applications



10

Add/Modify Form Layout

11.10.2023 Advancing Research Data Management with Python-Flask Applications



11

Search!

11.10.2023 Advancing Research Data Management with Python-Flask Applications



12

Add Shot

← → ↺

https://149.220.59.21:8080/tab1

80% ☆

🔍 📄 ☰

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

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

80% ☆

🔒 🔖 ⌵

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 Bulb: OFF

NF PM Bulb: 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

80% ☆

🔒

📄

☰

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 Shots in campaign: Go to Shot Number: Go

Shot identification

Shot Count: 5

This Shot

Date and Time

Laser parameters

GVD (fs^2)

Laser Energy (J)

Plasma Mirror? ☒

TW Intensity

TOD (fs^2)

TW Delay

Interaction parameters

TRO (deg)

TFO (μm)

Target details

Target (choices read from mediawiki) [\[LINK\]](#)

Post-shot readout

RamIon (μSv)

Proton Energy TPS 45 (MeV)

Proton Energy TPS 15 (MeV)

Time of flight (ns)

Proton Energy from TOF (MeV)

Measured GVD (fs^2)

Measured TOD (fs^2)

Comments:

Quality
OK
Bad
Calibration

Scan Type
E-Scan
GVD-Scan
TOD-Scan

Diagnostics

BS 0

BS -32

BS 20

CeramicCam

ColorCam TCC

FF after top DD

FF Spider

FF PM Bulli

NF PM Bulli

FTSI

ProtProf weak

ProtProf strong

Profiler3

Ref1 1w

Ref1 2w

Ref1 Spect

CosCorr

SPEBS 0

SPEBS -32

SPEBS 20

Spec Elec Prof

SPEm

XUV MCP

TPS 15

TPS 15 MCP

TPS 45

TPS 45 Lanex low

TPS 45 Lanex high

Trans Lanex

Trans 1w

Trans 2w

Trans Spect

Trans Spect 2w

Ge X spect

Ross Filter pair

SinglePhoton Spect

Diagn Shutter

FTSI Setup

Pickoff Att

ProtProf Setup

XUV Setup

Submit

Add/Modify Diagnostic Presets

ExperimentLog: Ions

Logged in as ktippeyLogoutAdmin Page

Add ShotModify ShotAdd/Modify Diagnostic PresetsAdd/Modify DiagnosticsAdd/Modify Form LayoutSearch!

Parameter fields

Diagnostics TypeBS 0

Clear Form

Name

Description

Set-up date:TT.MM.JJJJ

Details:

KeyValue

Responsible Person

PC (choices read from mediawiki)NONE ()

File path

Filename_schemaADD LATER

Counter_modeADD LATER

Submit

Add/Modify Presets for BS 0

Name	Description	Details	Responsible Person	PC	file_path	filename_schema	counter_mode	Set-up Date	Active	Clone	Modify	Delete
20220905 - now PCO edge	PCOedge 4.2 now with 12 mm and shielding	detector: acA1300-60gm, serial number: 23021477, delay time: 0, trigger: Ions5		fwk439 (Cameras TK Mini)		ADD LATER	ADD LATER	2022-09-05	<input checked="" type="checkbox"/>	Clone	Modify	Delete
20220901 - added Lanex	added lanex imaging	detector: acA1300-60gm, serial number: 23021477, delay time: 0, trigger: Ions5		fwk438 (Computer Fujitsu Primergy RX1330 m3)		ADD LATER	ADD LATER	2022-09-01	<input checked="" type="checkbox"/>	Clone	Modify	Delete
20220901 - changed distance	imaging Csl only, increased shielding, 7.8 cm to flanch	detector: acA1300-60gm, serial number: 23021477, delay time: 0, trigger: Ions5		fwk438 (Computer Fujitsu Primergy RX1330 m3)		ADD LATER	ADD LATER	2022-09-01	<input checked="" type="checkbox"/>	Clone	Modify	Delete
20220830 - CSI	imaging lanex stack spectrometer and Csl	detector: acA1300-60gm, serial number: 23021477, delay time: 0, trigger: Ions5		fwk438 (Computer Fujitsu Primergy RX1330 m3)		ADD LATER	ADD LATER	2022-08-30	<input checked="" type="checkbox"/>	Clone	Modify	Delete
20220830 - Pinhole further away	imaging lanex stack spectrometer and Csl, pinhole moved 1cm away from flanch	detector: acA1300-60gm, serial number: 23021477, delay time: 0, trigger: Ions5		fwk438 (Computer Fujitsu Primergy RX1330 m3)		ADD LATER	ADD LATER	2022-08-30	<input checked="" type="checkbox"/>	Clone	Modify	Delete
20220830 - Added shielding	imaging lanex stack spectrometer and Csl, pinhole moved 1cm away from flanch, added shielding	detector: acA1300-60gm, serial number: 23021477, delay time: 0, trigger: Ions5		fwk438 (Computer Fujitsu Primergy RX1330 m3)		ADD LATER	ADD LATER	2022-08-30	<input checked="" type="checkbox"/>	Clone	Modify	Delete
init	init	detector: acA1300-60gm, serial number: 23021477, delay time: 36		fwkmg123 (Tower)		ADD LATER	ADD LATER	2022-08-24	<input checked="" type="checkbox"/>	Clone	Modify	Delete
20220826 - imaging lanex	imaging lanex stack spectrometer	detector: acA1300-60gm, serial number: 23021477, delay time: 0, trigger: Ions5		fwk438 (Computer Fujitsu Primergy RX1330 m3)		ADD LATER	ADD LATER	2022-08-24	<input checked="" type="checkbox"/>	Clone	Modify	Delete
OFF	offline			NONE ()		ADD LATER	ADD LATER		<input checked="" type="checkbox"/>	Clone	Modify	Delete

12 11.10.2023 Advancing Research Data Management with Python-Flask Applications

DAPHONE
4NFOI

HMC

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concept
SCIENCE AND
INNOVATION CAMPUS

HZDR

Add/Modify Diagnostics

ExperimentLog: Ions

[Add Shot](#) [Modify Shot](#) [Add/Modify Diagnostic Presets](#) [Add/Modify Diagnostics](#) [Add/Modify Form Layout](#) [Search!](#)

Add New

Display Name: BS 0

Tooltip Description: Bremsstrahlung Bulbi in laser forward direction <serial numbers, ...>

Details: Bremsstrahlung Bulbi in laser forward direction <serial numbers, ...>

Class:

Wiki-Link(s):

Team: Ions

Responsible:

Valid since: TT. MM. JJJJ

Valid until: TT. MM. JJJJ

Submit

Available Diagnostics

Display Name	Tooltip Description	Details	Class	Wiki-Link(s)	Team	Responsible	Valid since	Valid until	Clone	Modify
BS 0	Bremsstrahlung Bulbi in laser forward direction <serial numbers, ...>	Bremsstrahlung Bulbi in laser forward direction <serial numbers, ...>			Ions		None	None	Clone	Modify
BS -32	Bremsstrahlung Bulbi at -32° (more in target plane)	Bremsstrahlung Bulbi at -32° (more in target plane)			Ions		None	None	Clone	Modify
BS 20	Bremsstrahlung Bulbi at +20° (more target normal)	Bremsstrahlung Bulbi at +20° (more target normal)			Ions		None	None	Clone	Modify
CeramicCam					Ions		None	None	Clone	Modify
ColorCam TCC	Color Cam looking at TCC				Ions		None	None	Clone	Modify
FF after top DD	Farfield at upper DD mirror				Ions				Clone	Modify
FF Spider	Farfield at spider diagnostic				Ions				Clone	Modify
FF PM Bulbi	Farfield at Plasmamirror Bulbi				Ions				Clone	Modify
NF PM Bulbi	Nearfield at Plasmamirror Bulbi				Ions				Clone	Modify
FTSI			1D		Ions		None	None	Clone	Modify
ProtProf weak					Ions		None	None	Clone	Modify
ProtProf strong		DETAILS			Ions		None	None	Clone	Modify
Profiler3					Ions				Clone	Modify
Refl 1w					Ions				Clone	Modify
Ref 2w		DETAILS			Ions		None	None	Clone	Modify

Add/Modify Form Layout

← → ↺

🔒 https://149.220.59.21:8080/select_choices

80% ☆

🔒 📄 ☰

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!](#)

Adjust/add new template

APPLY TEMPLATE

Select template:

Something Different

Name your template:

Something Different

Team:

Campaign:

NONE

Details:

Set-up date:

10.08.2023

Choices:

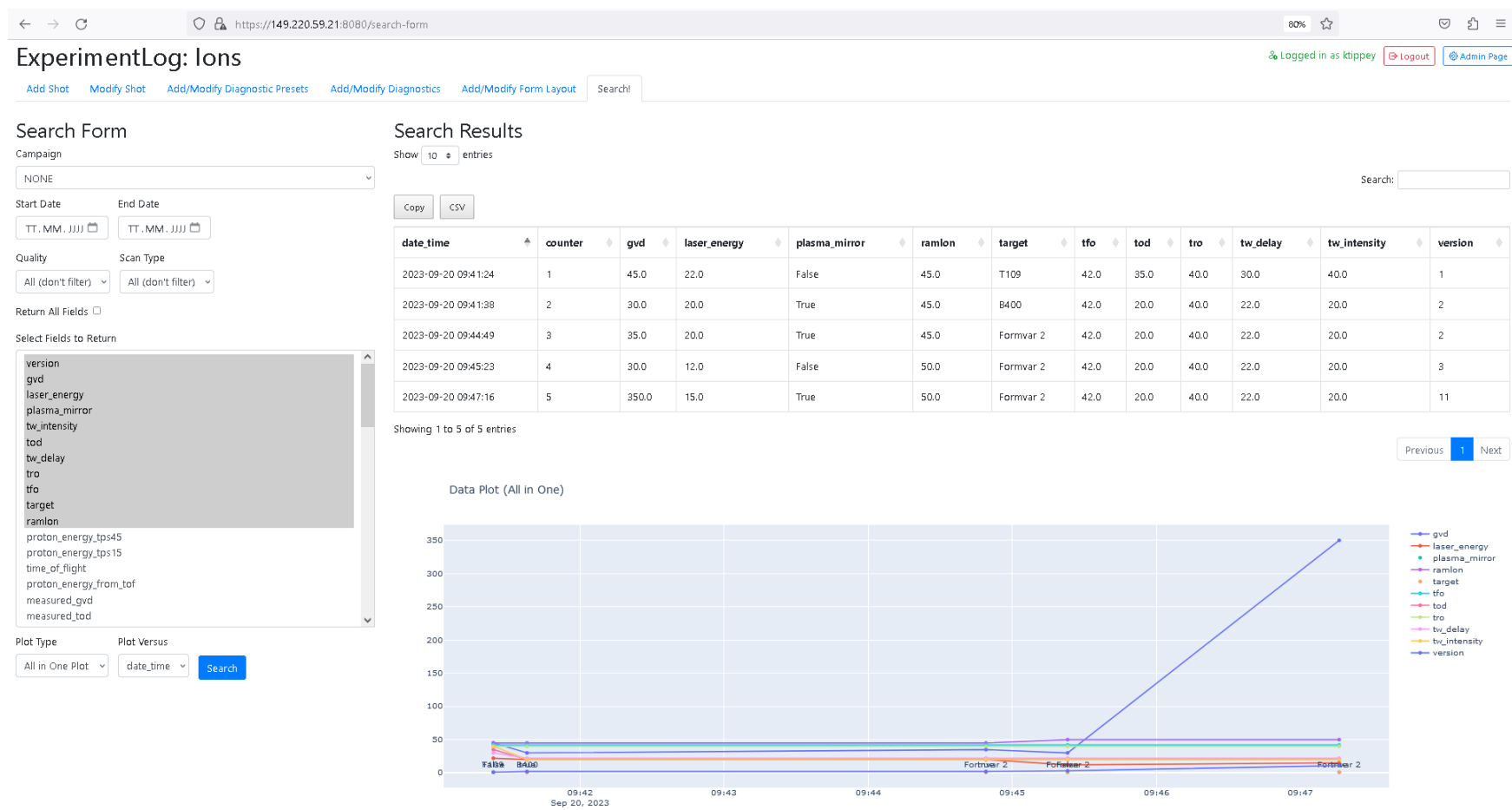
FF after top DD
FF Spider
FF PM Bulli
NF PM Bulli
FTSI
ProtProf weak
ProtProf strong
Profiler3
Refi 1w
Refi 2w
Refi Spect
CosCorr
SPEBS 0
SPEBS -32
SPEBS 20
Trans 1w
Trans 2w
Ross Filter pair
Pickoff Att

Save

Available Templates

Template Name	Team	Campaign	Details	Set-up Date	Active	Delete
Something Different		NPL Dosimetry 12.2022 (2022-12-12 to 2022-12-16)		2023-08-10	<input checked="" type="checkbox"/>	Delete
Template of the Year	Electrons	EMP-Birdhouse 11.2022 (2022-12-12 to 2022-12-16)	All the best details	2023-07-06	<input checked="" type="checkbox"/>	Delete
All Fields	TEAM		DETAILS	2022-09-01	<input checked="" type="checkbox"/>	Delete
All + recent additions		NONE 0		None	<input checked="" type="checkbox"/>	Delete

Search!



Shotsheet [electrons]: The different tabs

Outline

Electron Shot Form

Shot Details: Shot Number (18), Shot Length (10), Comments and Flags (107140-123), Laser Field (107140-123), Laser Quality Check (Very Good).

Laser Parameters: Laser Wavelength (107140-123), Laser Pulse Numbers (107140-123), Laser Field (107140-123), Laser Quality Check (Very Good).

Target Parameters: Target Type (107140-123), Bottom Target Type (107140-123), Bottom Target Depth (107140-123), Bottom Target Pressure (107140-123).

Diagnostics Settings: Epile Position (107140-123), Epile Position (107140-123), Epile Position (107140-123), Epile Position (107140-123).

Advanced Settings: Top View Filter Value (107140-123), Side View Filter Value (107140-123), Over View Filter Value (107140-123), Under View Filter Value (107140-123).

Electron Shot Form

Laser Parameters: Laser Wavelength (107140-123), Laser Pulse Numbers (107140-123), Laser Field (107140-123), Laser Quality Check (Very Good).

Target Parameters: Target Type (107140-123), Bottom Target Type (107140-123), Bottom Target Depth (107140-123), Bottom Target Pressure (107140-123).

Diagnostics Settings: Epile Position (107140-123), Epile Position (107140-123), Epile Position (107140-123), Epile Position (107140-123).

Advanced Settings: Top View Filter Value (107140-123), Side View Filter Value (107140-123), Over View Filter Value (107140-123), Under View Filter Value (107140-123).

Select Fields

Select a Form Layout or Make a New One

Available Layouts:

Layout Name	Description	Responsible Person	Action
Existing Fields	Existing Fields	IT	View
New Fields	New Fields	IT	View
Existing Fields	Existing Fields	IT	View

Select Fields to Display:

Available Fields:

- Shot Number
- Shot Length
- Comments and Flags
- Laser Field
- Laser Quality Check
- Target Type
- Bottom Target Type
- Bottom Target Depth
- Bottom Target Pressure
- Epile Position
- Top View Filter Value
- Side View Filter Value
- Over View Filter Value
- Under View Filter Value

Add a New Field

Add New Field

Existing Custom Fields:

Field Name	Details	Device	Field Type	Action
New Field	New Field	Shot Details	String	View
New Field	New Field	Shot Details	Float	View
New Field	New Field	Shot Details	Quality	View

Add New Field:

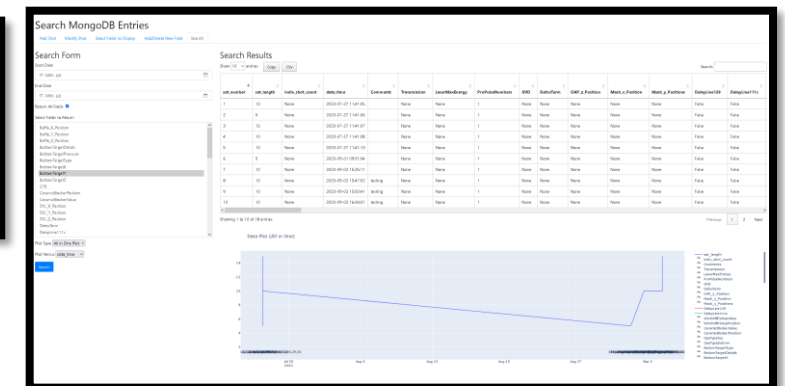
Field Name: [Text Field]

Details: [Text Field]

Device: [Text Field]

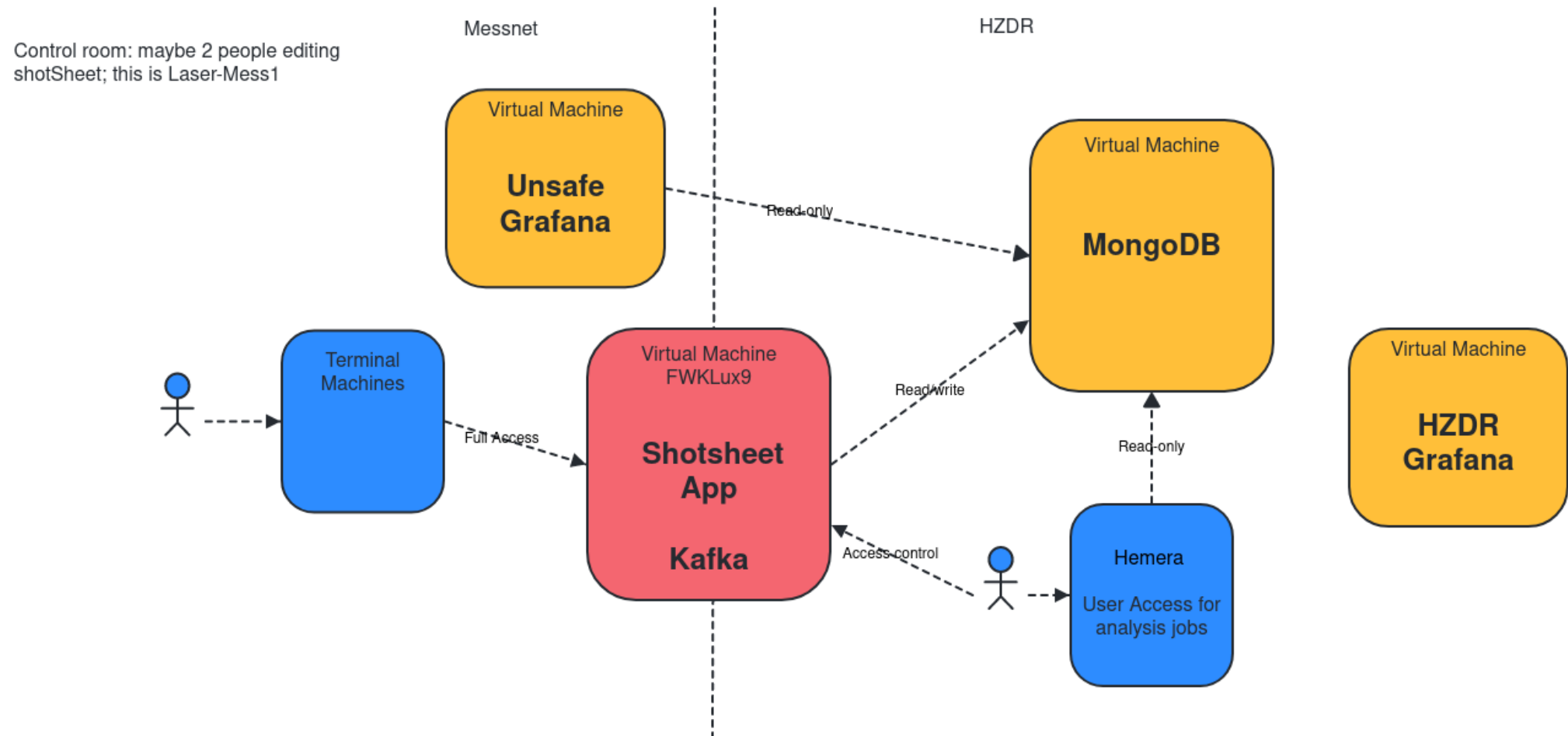
Field Type: [Text Field]

Action: [Text Field]



Shotsheet: Basic Setup

Planned deployment implementation



Demo?

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

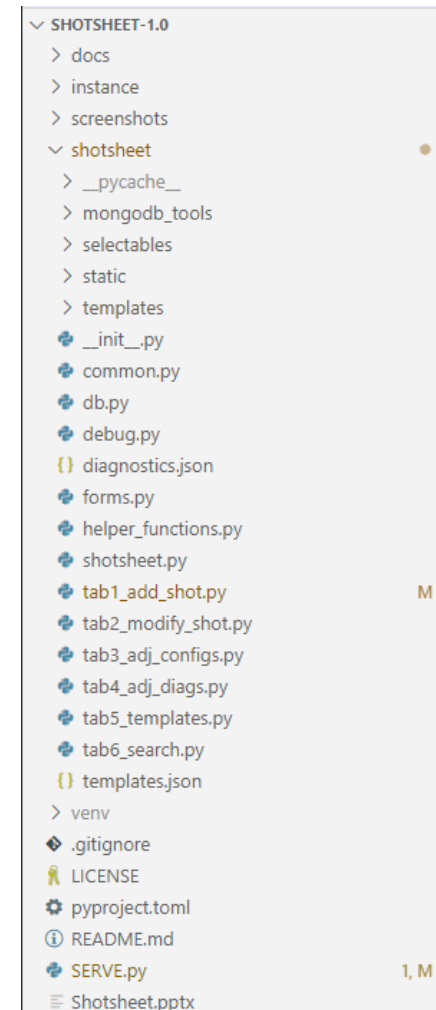
IONS*

<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

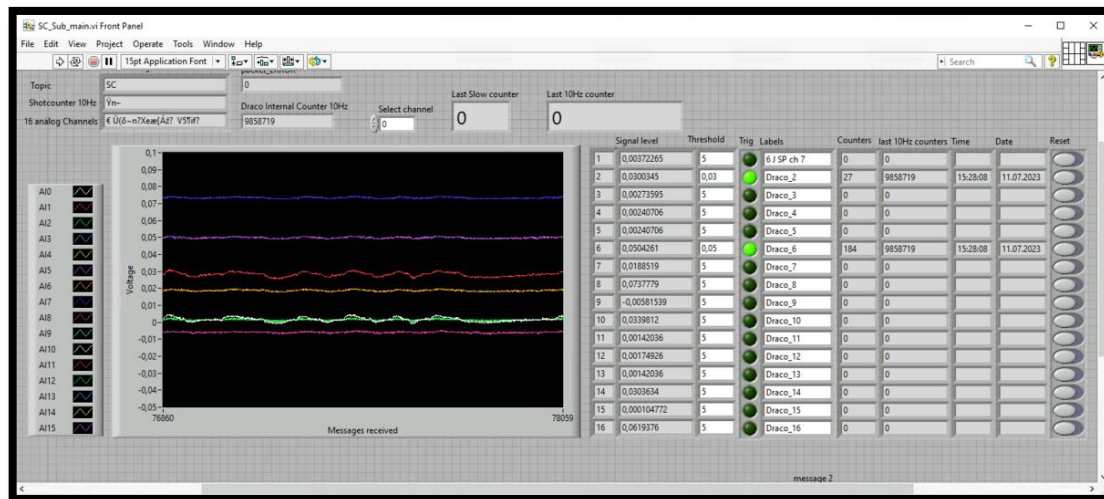
Labview ZeroMQ Relay

No ability to message out with Kafka
Complicated license situation

->

Python Flask ZeroMQ Relay

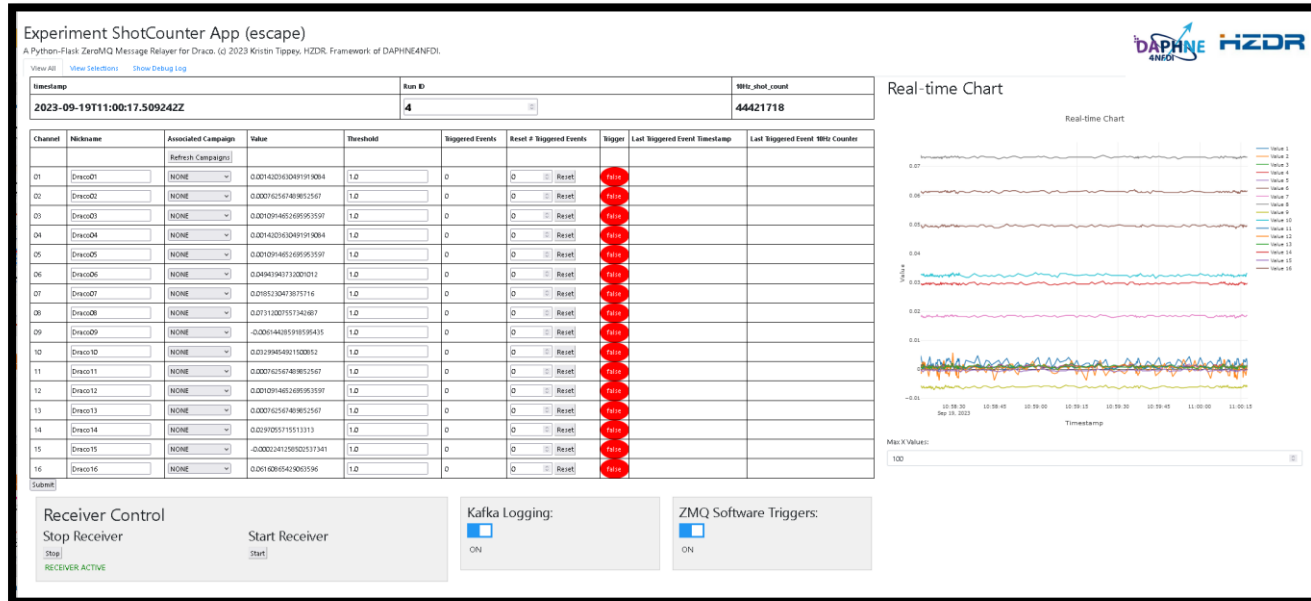
Able to message directly out with Kafka
No license issues



LabView Credit: Wolfgang Horn

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

ZeroMQ Relay: Main page, selection page, debug page

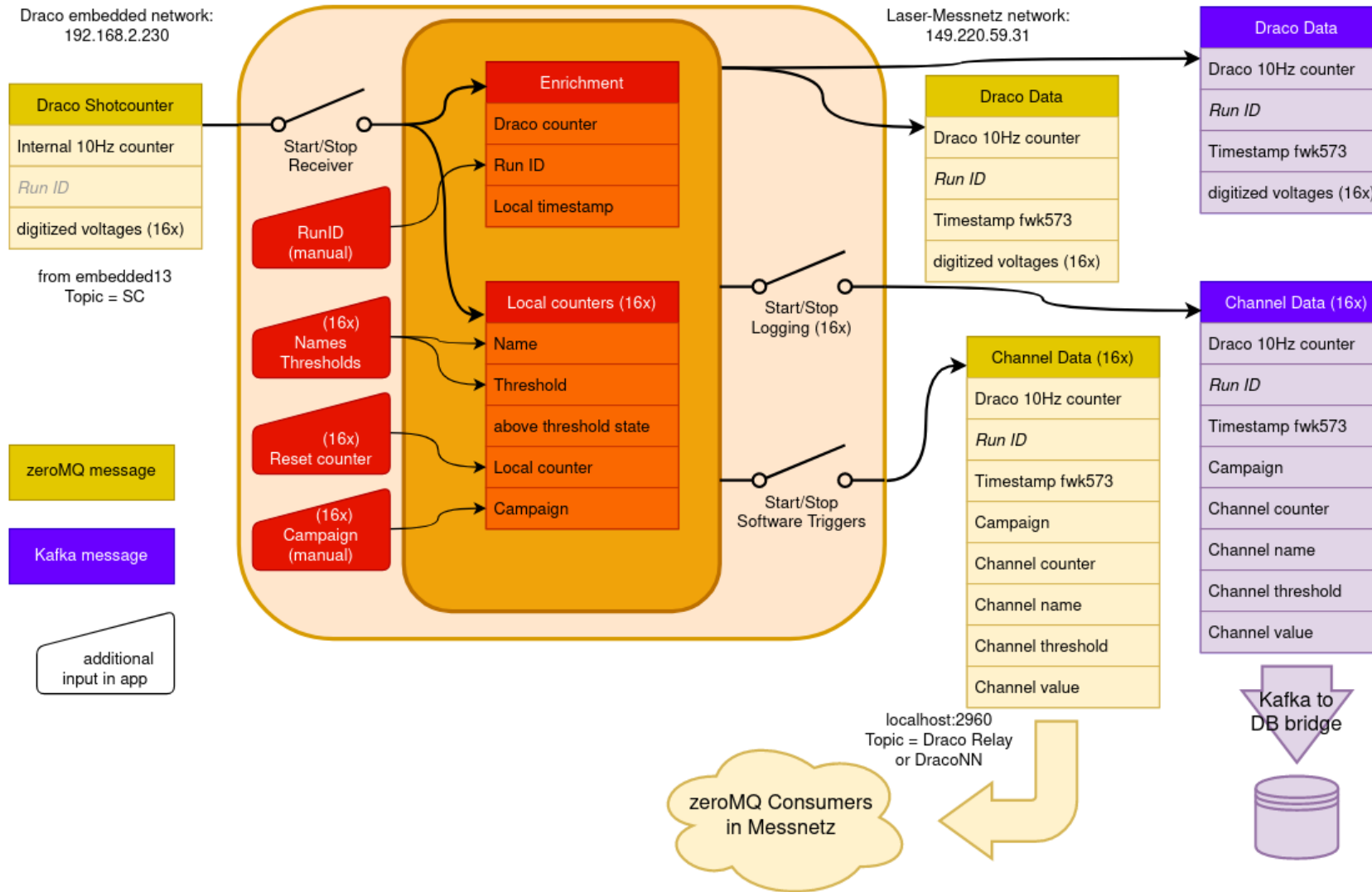


- Displays incoming ZeroMQ data in tabular and graphical form
- User input of nicknames, campaigns, thresholds, local trigger counts
- Triggers upon incoming values > threshold values
- Relays **triggered data** to Kafka (MongoDB) and **all data** to ZeroMQ (future: software triggers)

Demo?

<http://149.220.59.31:8888/>

Experiment ShotCounter and enrichment app (escape)



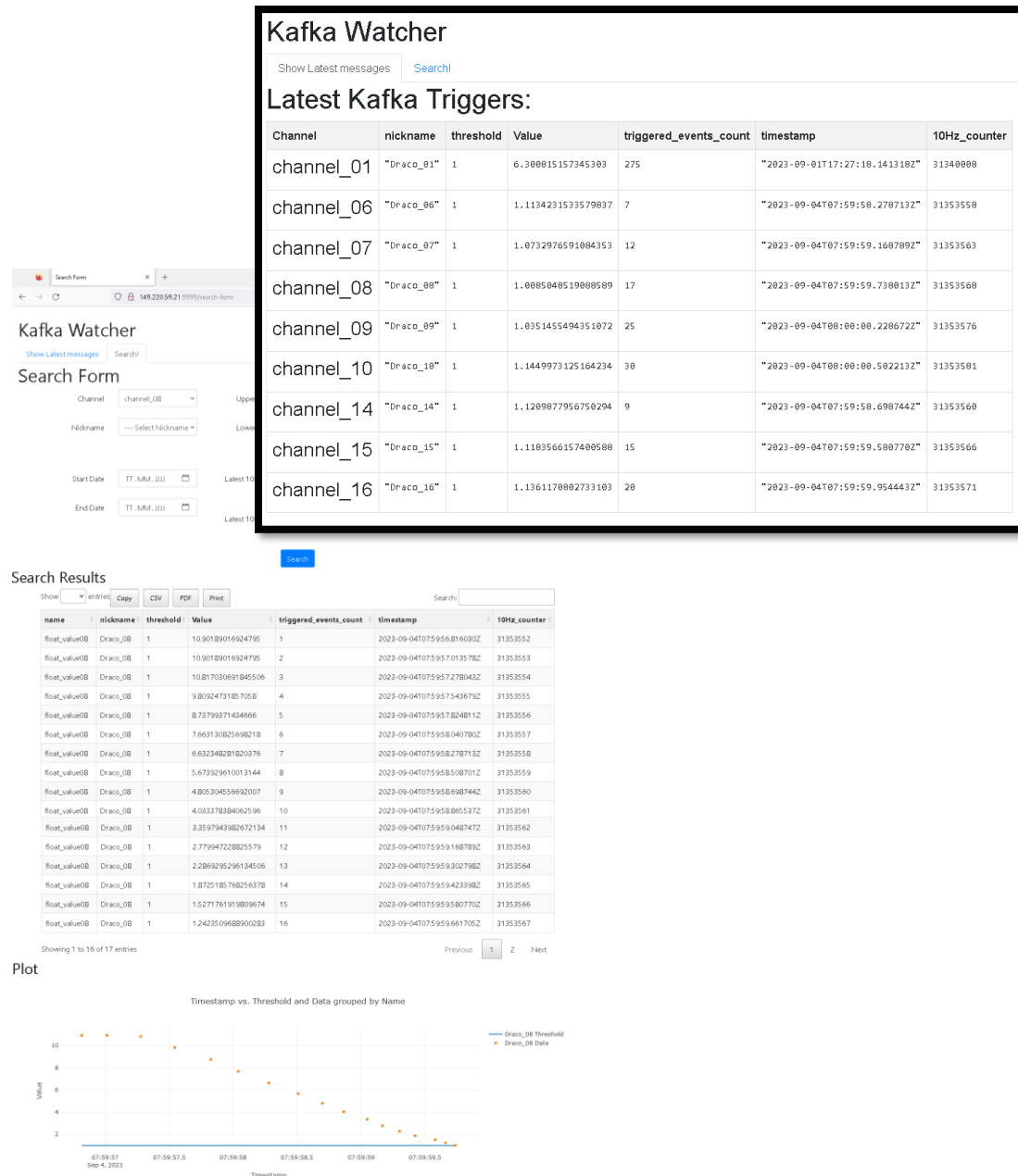
Kafka Receiver and Relay to MongoDB

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

Specifics:

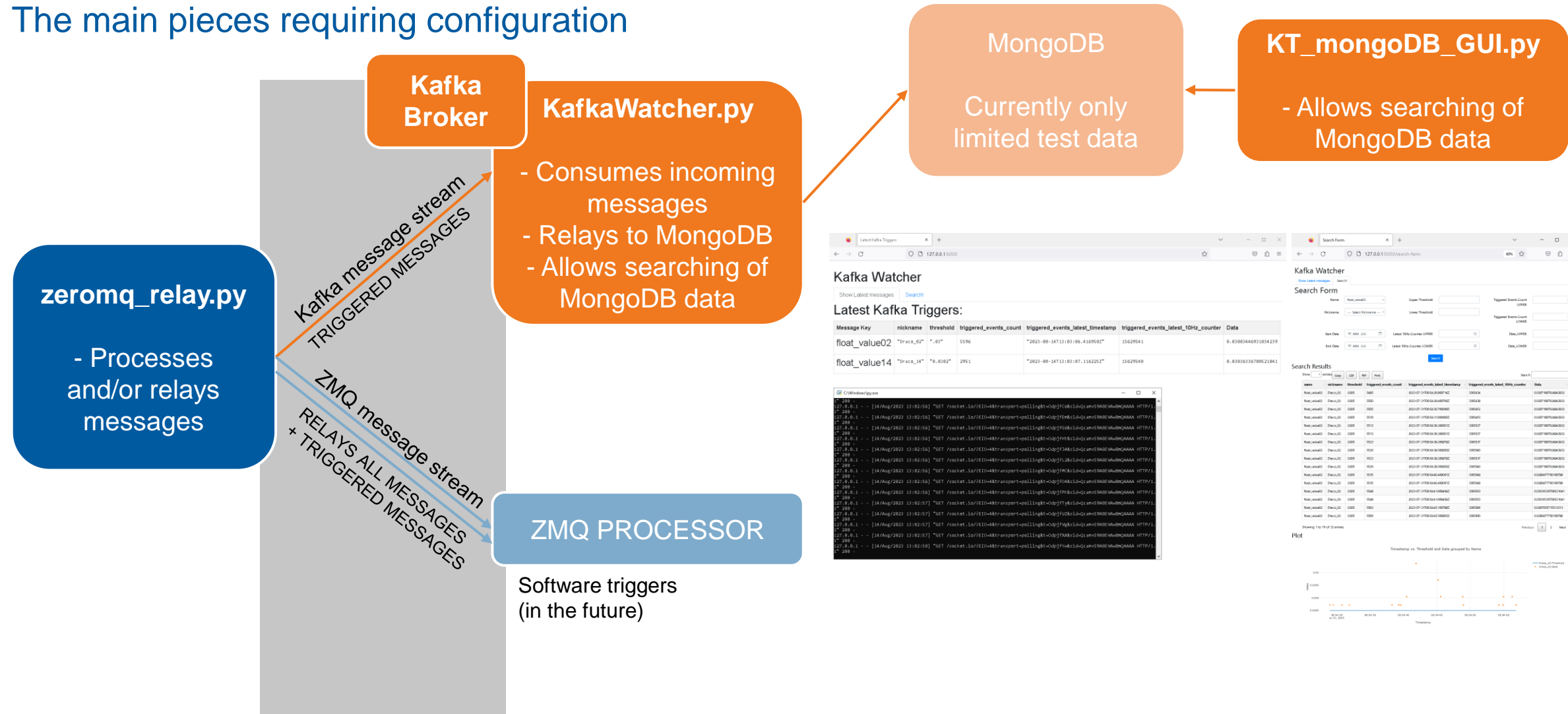
- Connected to kafka broker on fwklux9
- Serve KafkaWatcher from fwklux9 with:

```
unicorn --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/>

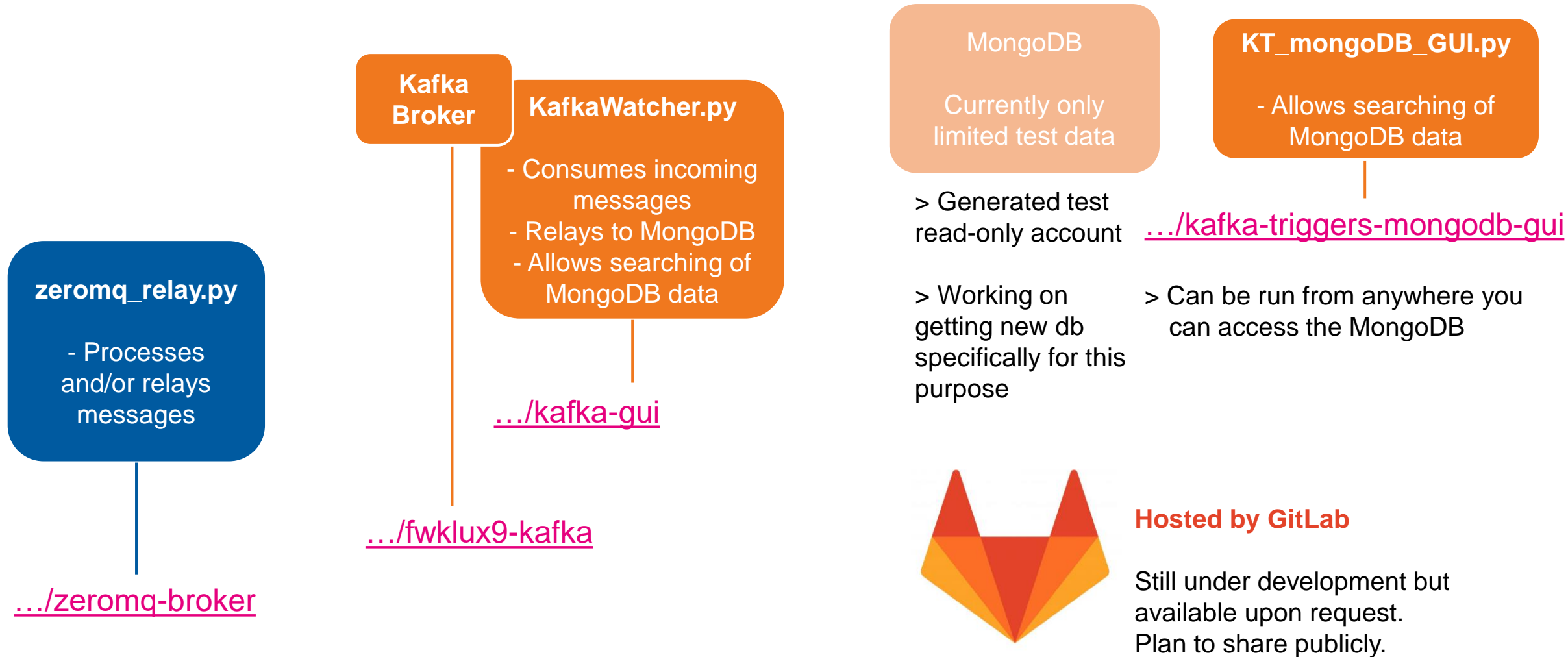


ZeroMQ Relay and KafkaWatcher: Basic Setup

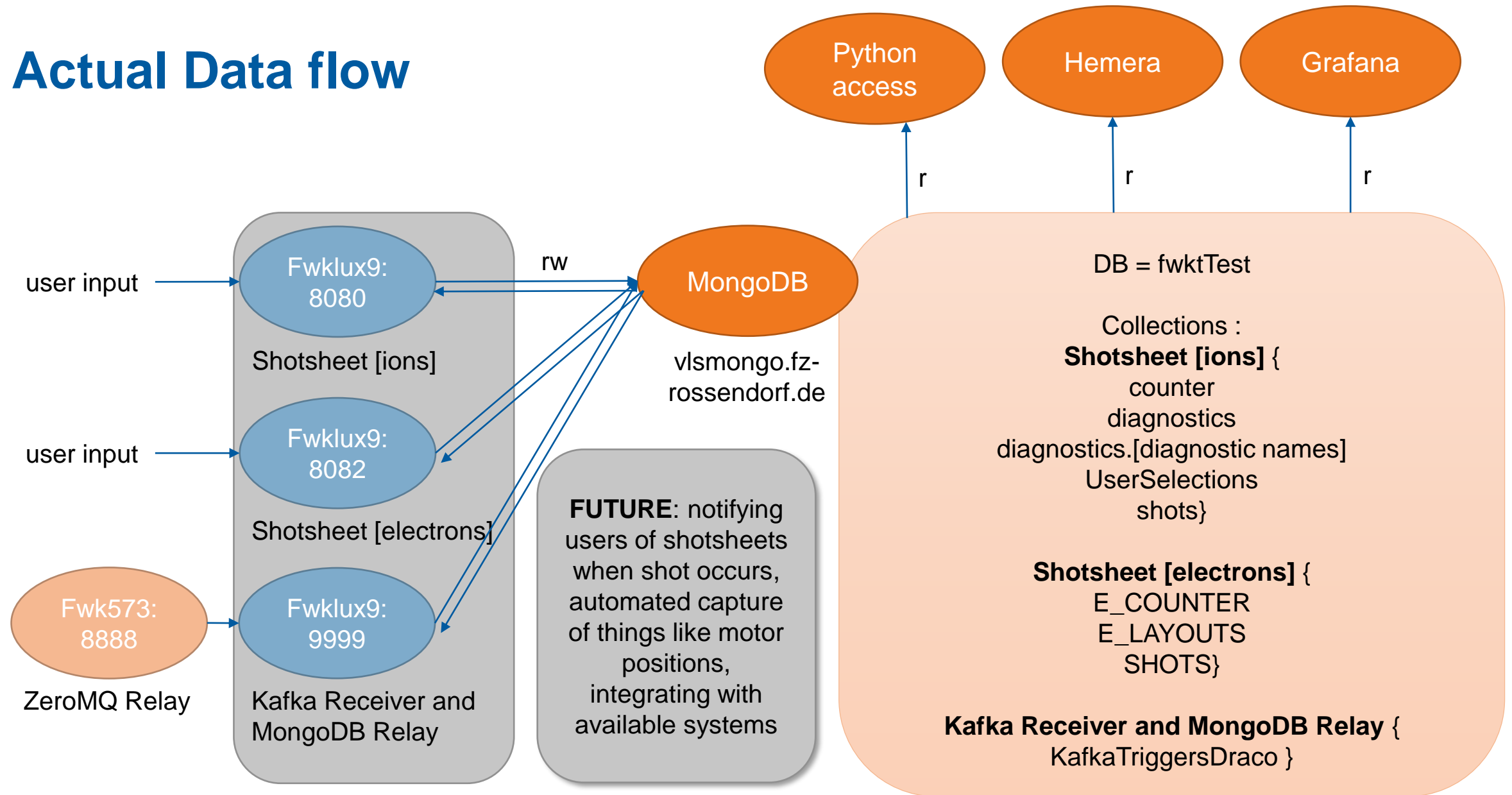
The main pieces requiring configuration



ZeroMQ Relay and KafkaGUI: Where to get the different pieces



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?

The screenshot shows the SciCat web interface. The top navigation bar includes 'Help', 'About', and 'Sign in'. The main content area displays details for a dataset with ID 'HZDR/8c5a4021-e2c5-43b4-8686-87d91fef6fc5'. The 'General Information' section includes fields for Name, Description, PID, Type, Creation Time, and Keywords. The 'Creator Information' section lists Owner, Principal Investigator, Orcid, Contact Email, Owner Group, and Access Groups. The 'Related Documents' section shows Creation Location and Techniques. A 'Scientific Metadata' section is partially visible. On the right, a visualization shows a cross-section of a simulation with a legend for 'Aluminum-Oxygen' and 'Aluminum'.

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 educate ingesters 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

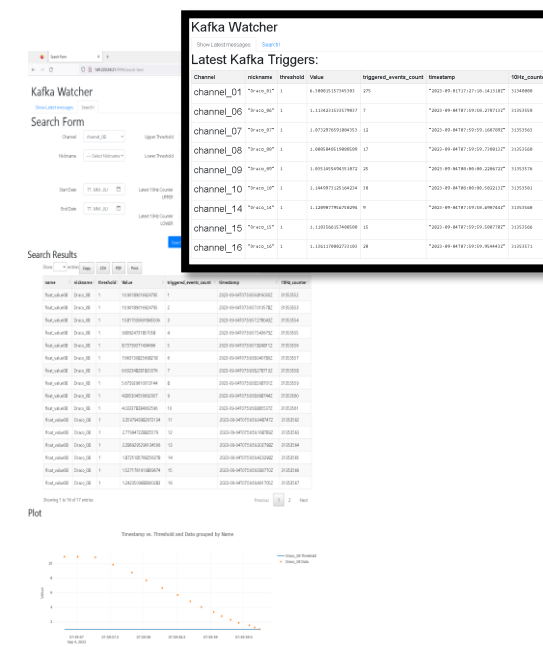
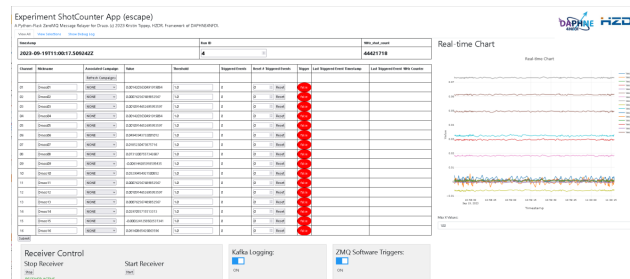
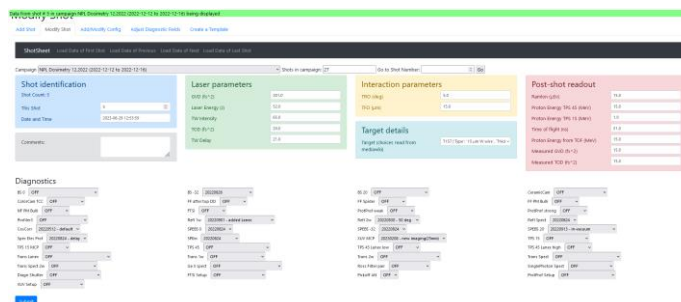
Shotsheet [ions] <https://149.220.59.21:8080/>
and **[electrons]** <https://149.220.59.21:8082/>

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

Smile:) PIconGPU

