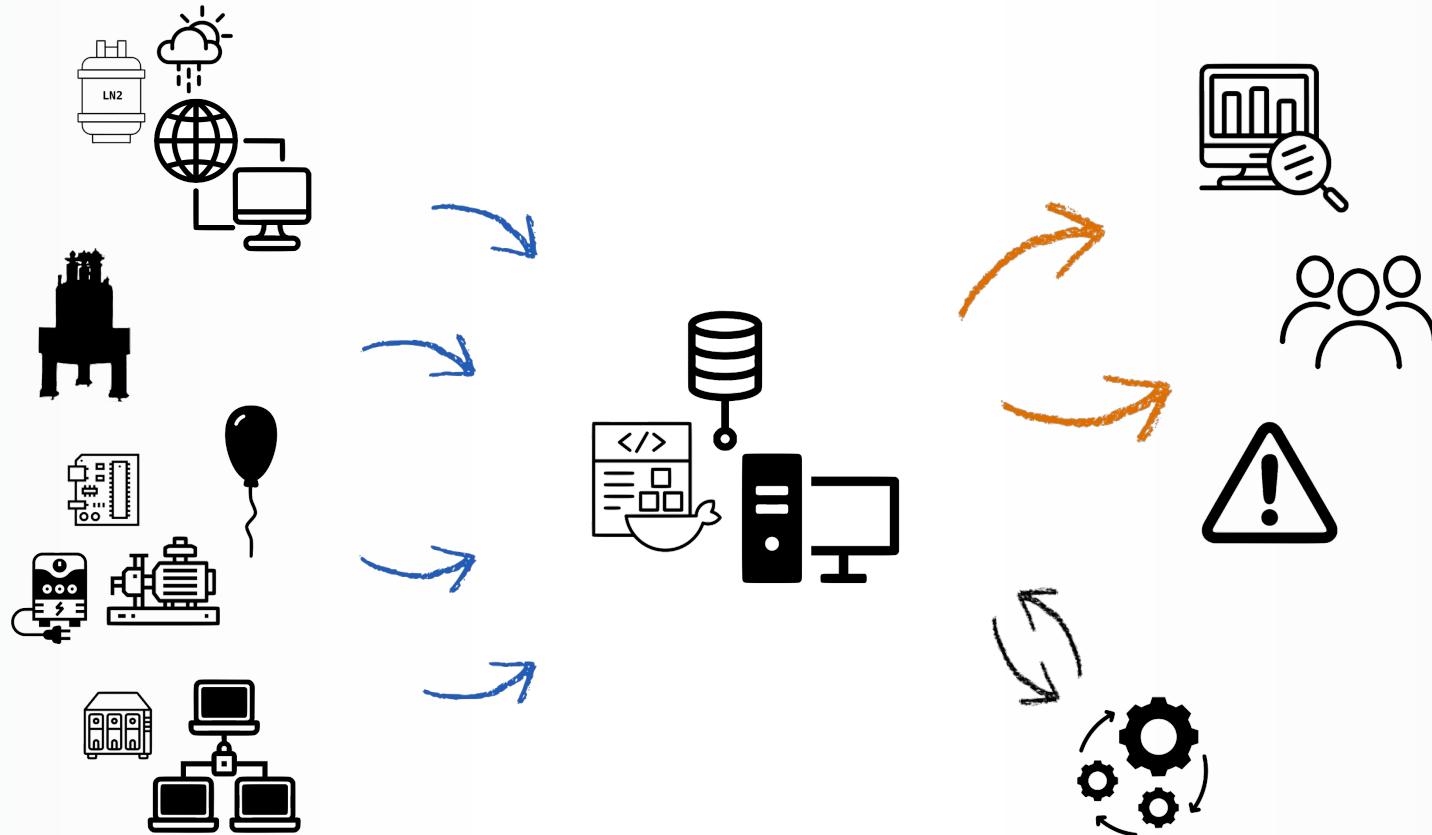


NMR Laboratory Monitoring



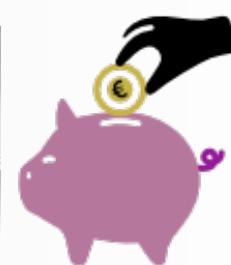
James Tolchard

24th August 2023

Why ?



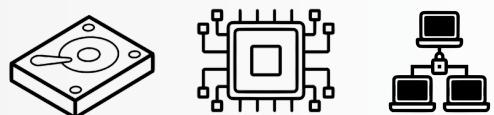
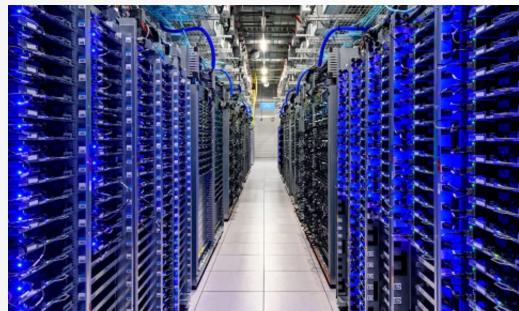
- Network Connectivity Issues



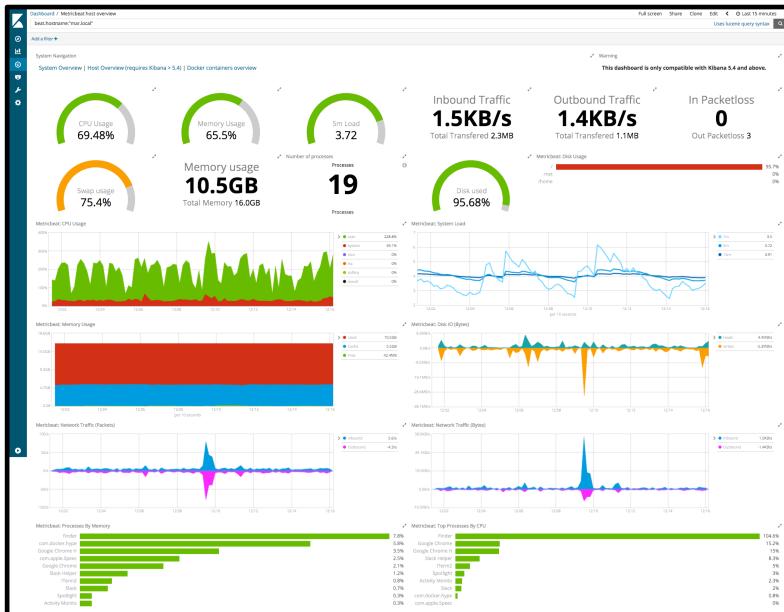
- Quantitative Evaluation of Helium Recycling

Inspiration

EMBL-EBI



Resource Dashboard



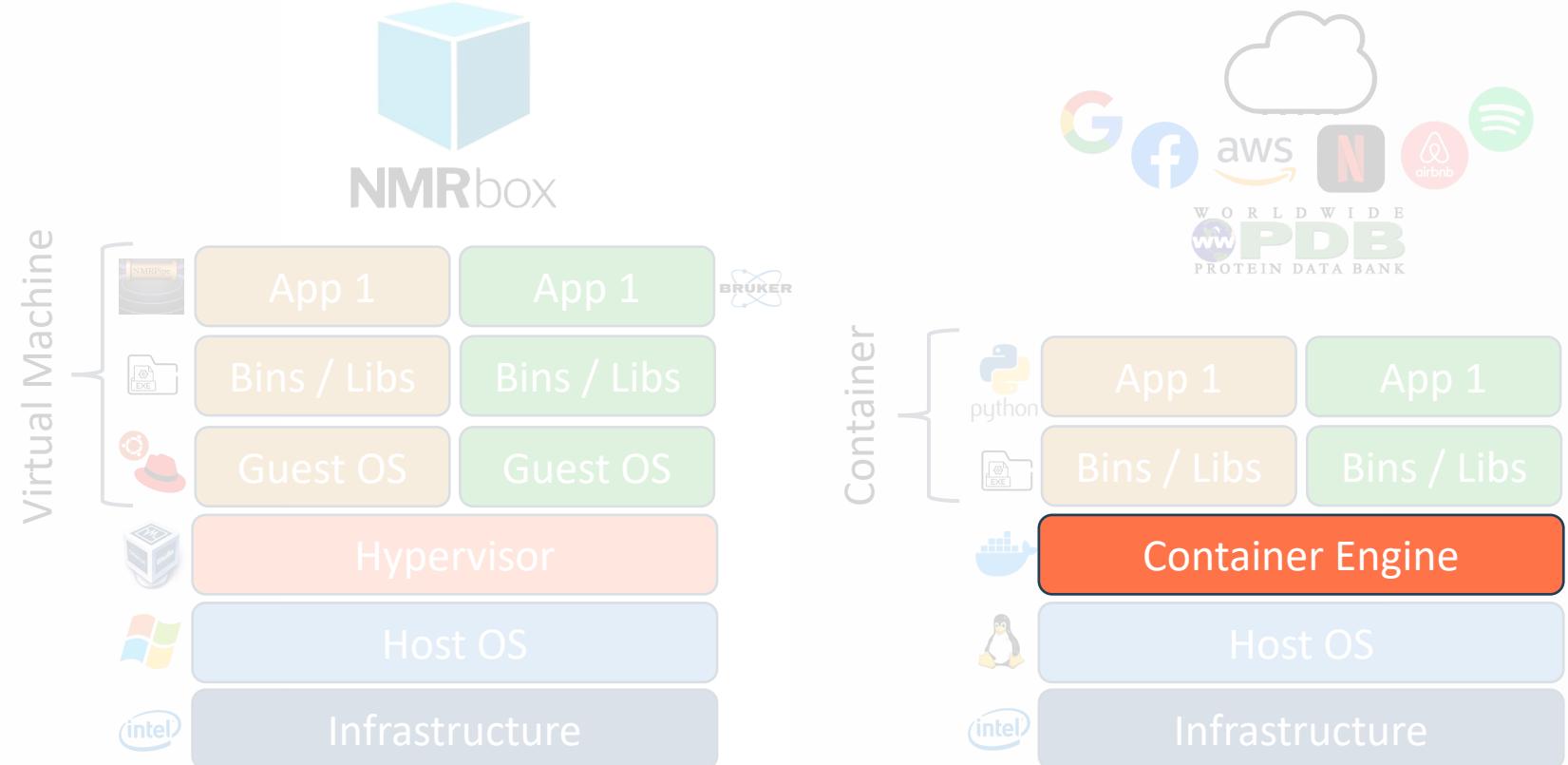
- Helps troubleshooting
 - Problems / correct departments
- Long-term trends
- Metric triggers
 - Preemptive-intervention
 - Alerts:
 - Automated comms. (Email/Slack)
 - Scriptable reactions



How ? - Containerization

Key requirements

- Scalable
- Cross-platform
- Low Overheads
- Fast
- Free
- Easy to develop



How ? - Containerization

Container Engines / Platforms

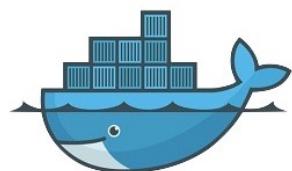


AWS ECS

+ more...

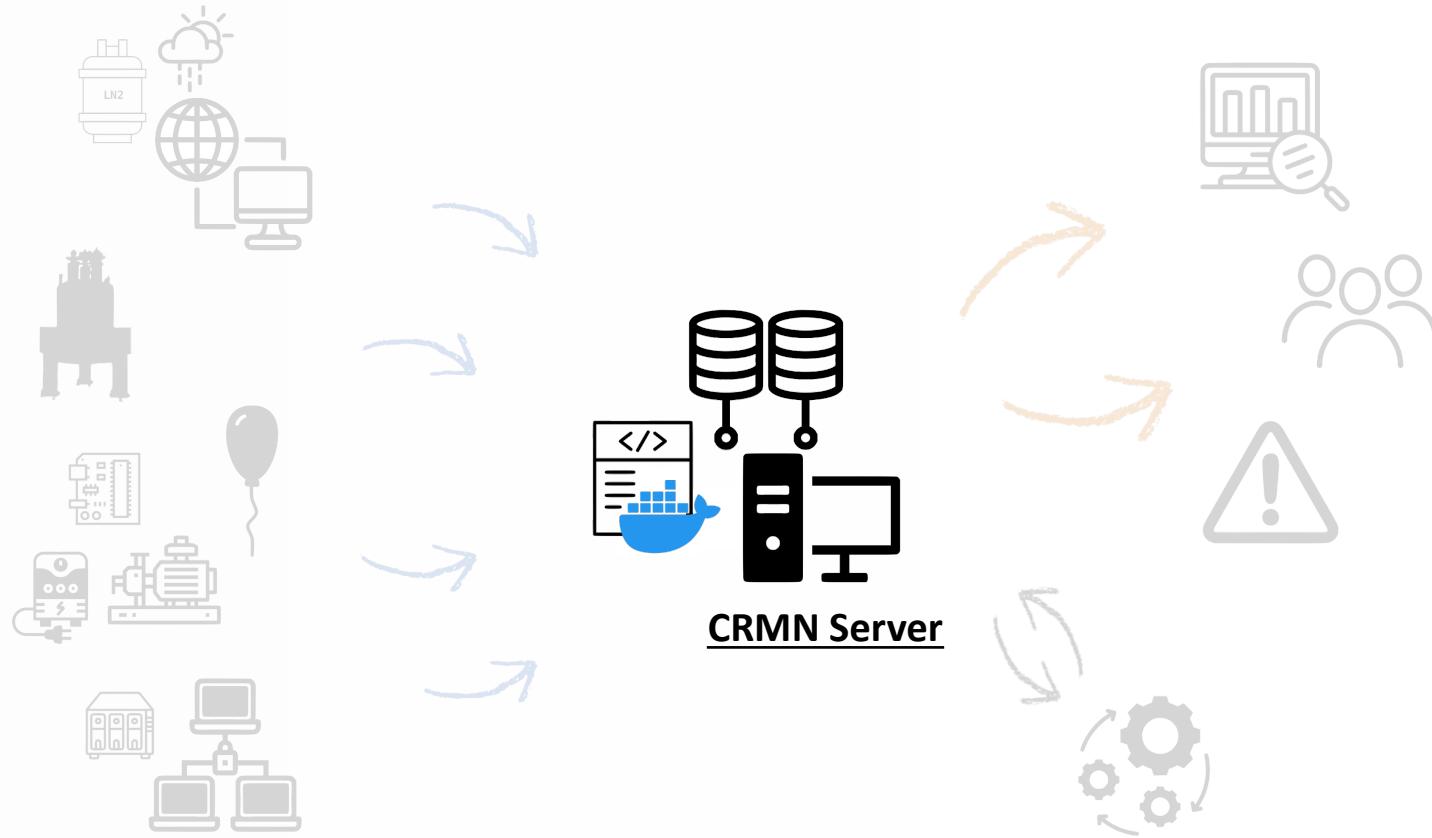
- Simple / User friendly CLI
- Easy to Develop
- Straightforward local installation
- Community / Documentation / Support
- Open source (core) & free to use
- Vast Eco-system (100,000+ images)

Docker Hub



SCANS

Simple Containerized Analysis for NMR Systems



Containers



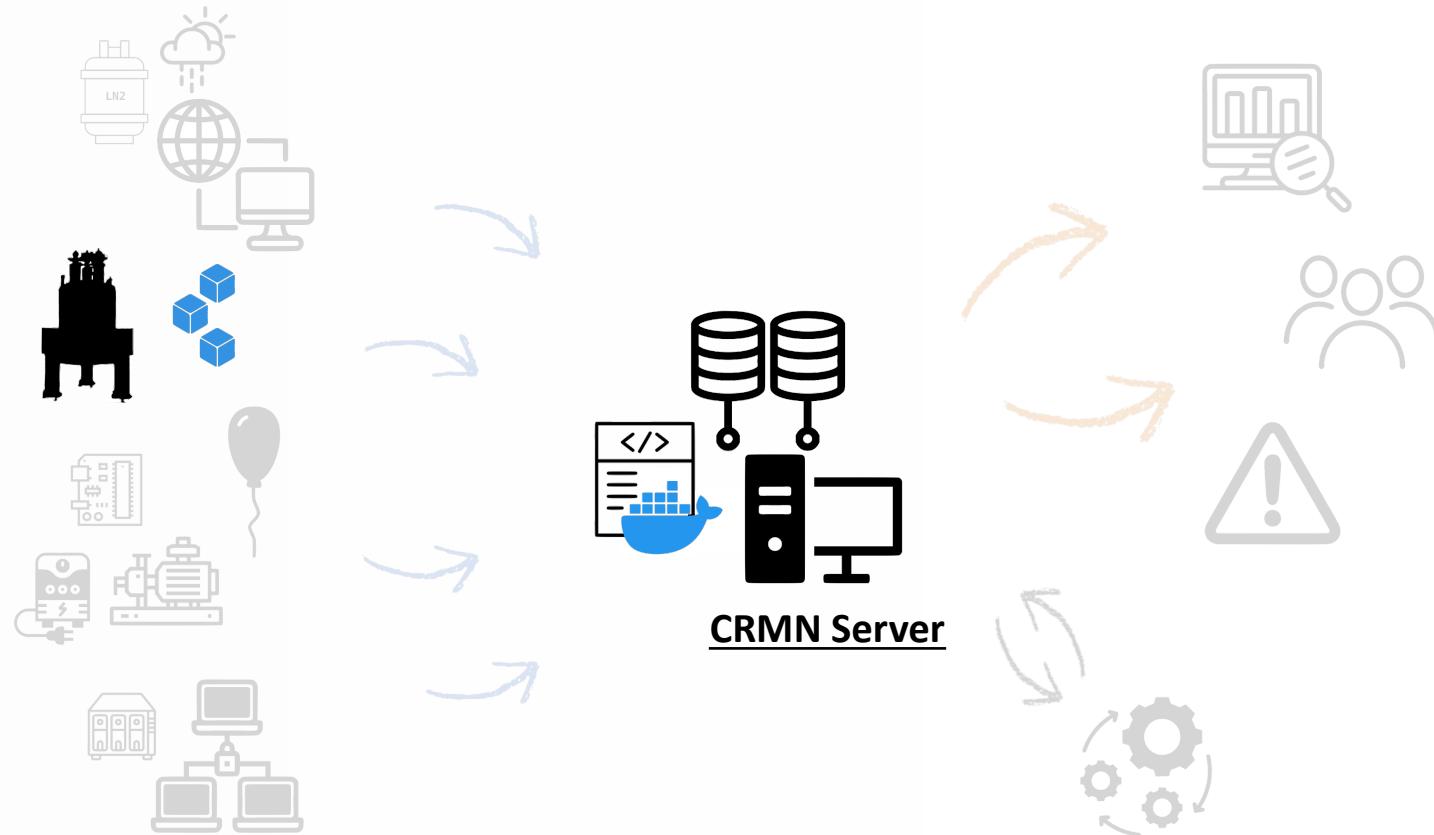
Prometheus

Time-Series database

- Scrapes data over HTTP
 - Fixed retention time per DB
1. Cryogen metrics (low res., 2-year retention)
 2. Computer metrics (high res. 2-week retention)

SCANS

Simple Containerized Analysis for NMR Systems



Spectrometer containers

Node Exporter

- Collects computer metrics
-

Spectrometer

- Collects MICS metrics
-



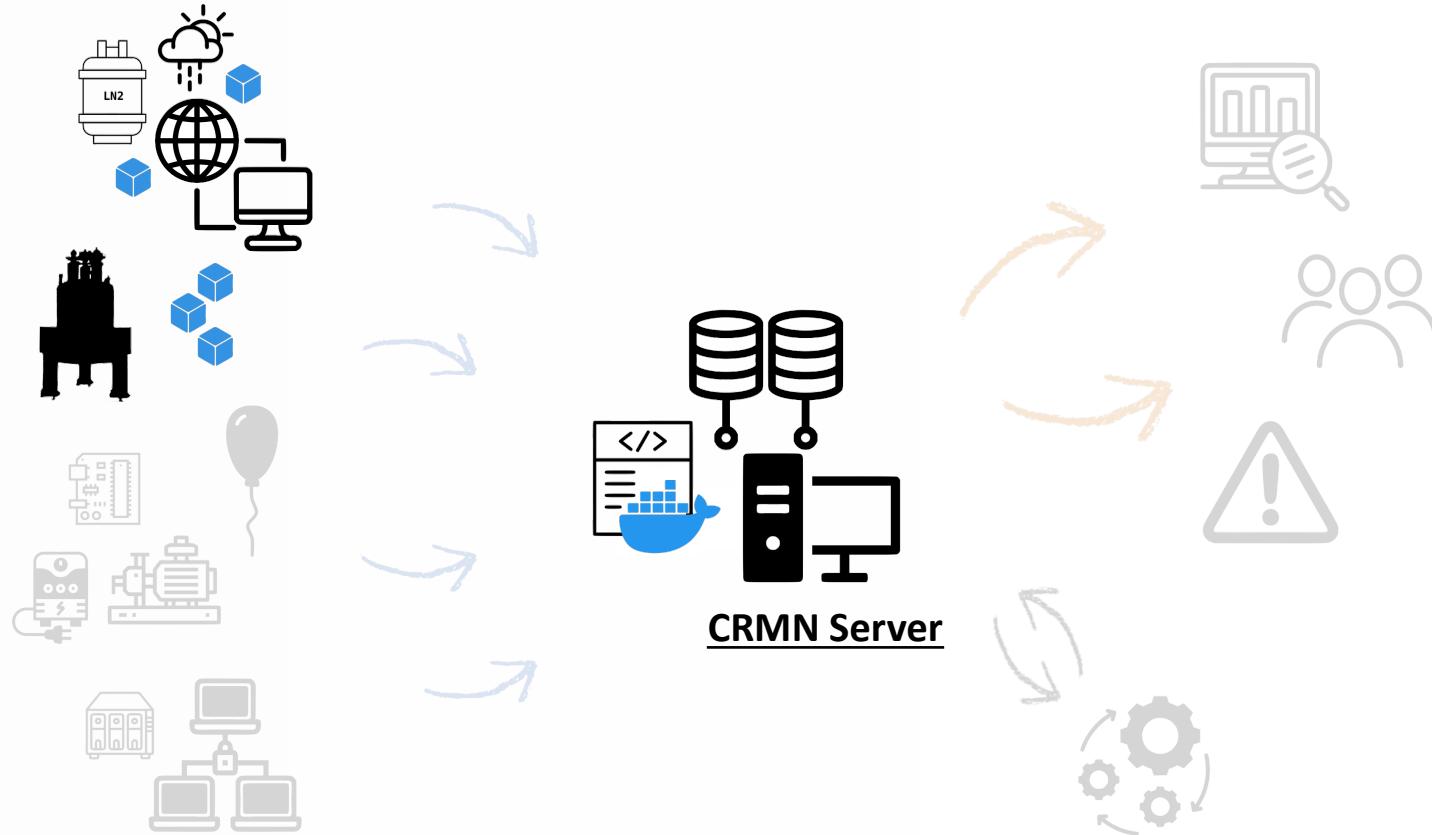
Non-MICS cryogens

- Checks HLMU readings
-



SCANS

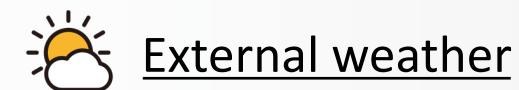
Simple Containerized Analysis for NMR Systems



Web-scraping containers



Accesses Air Liquide APIs
for Tank & SPI information



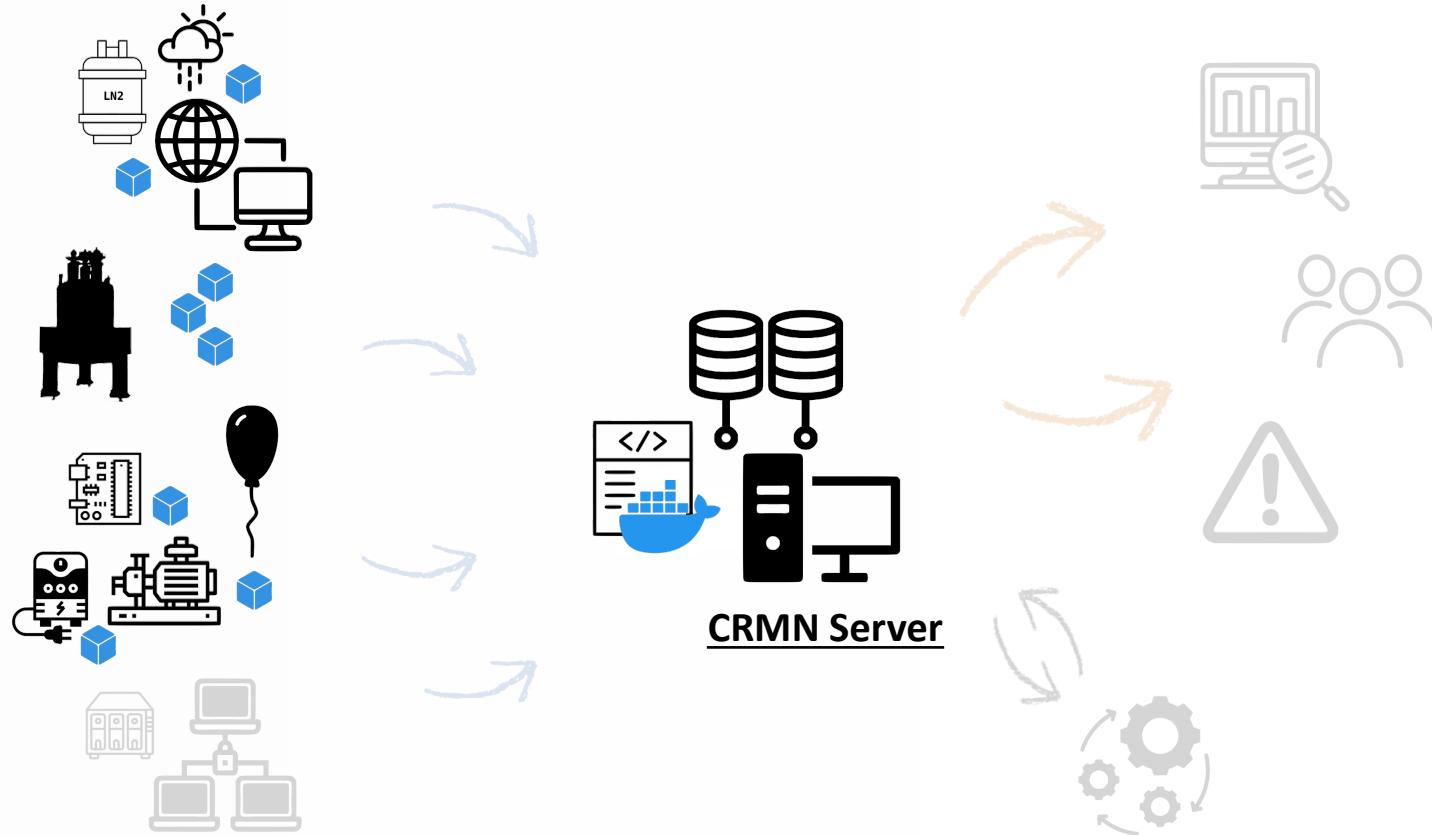
External weather

Monitors external
conditions via API



SCANS

Simple Containerized Analysis for NMR Systems



Hardware-scraping containers



Compressor info

- Python script creates logs via ModBus comm.



UPS info

- Scrapes UPS details via local web-interface



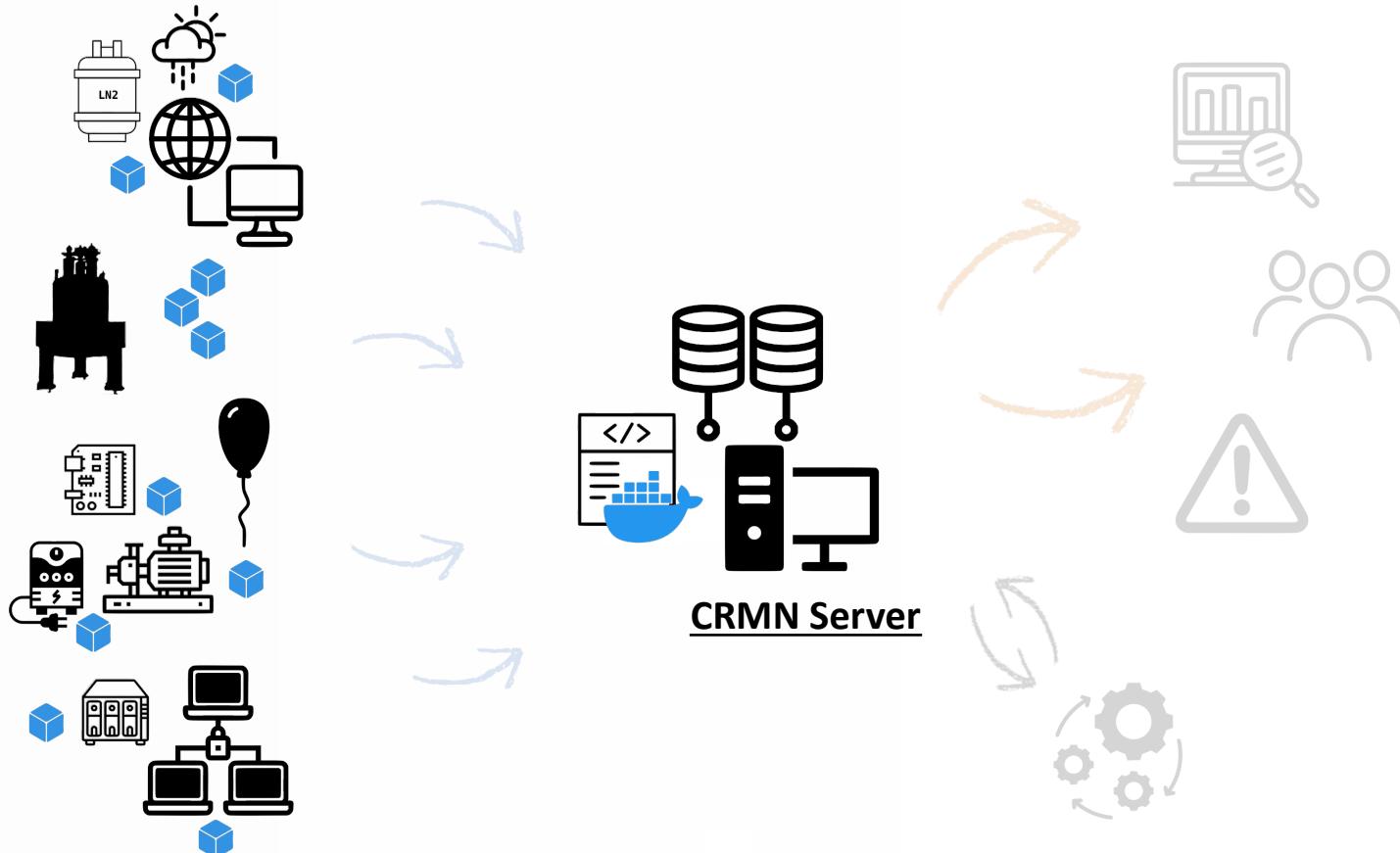
NMR Hall Env. sensor

- Temp, humidity & pressure via custom Arduino API



SCANS

Simple Containerized Analysis for NMR Systems



Hardware-scraping containers



Dell Server Metrics

- RAID Storage metrics

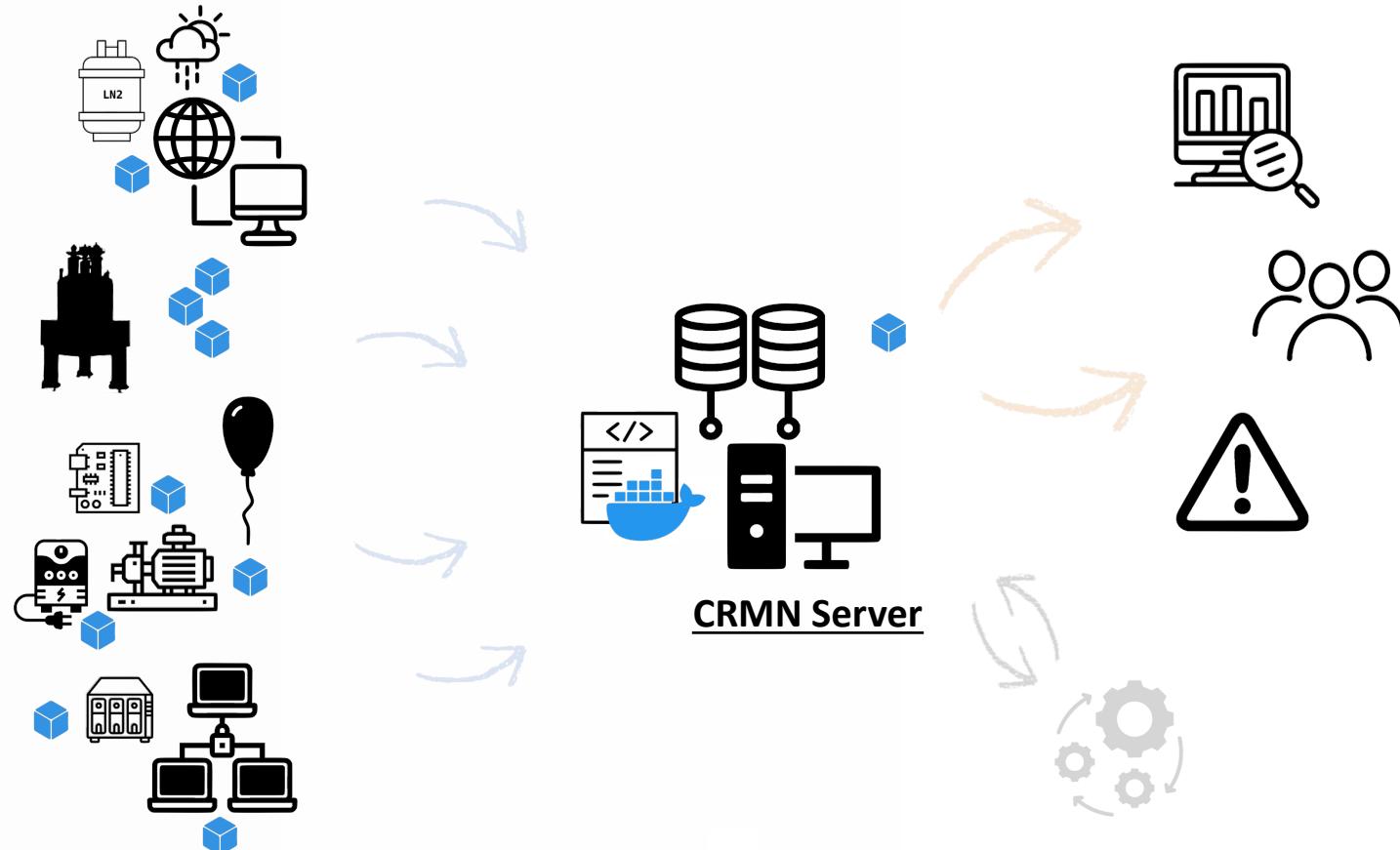


Blackbox exporter

- Analyses network response times

SCANS

Simple Containerized Analysis for NMR Systems



Visualization & analysis container



Grafana

- Query Prometheus DBs and create interactive charts and dashboards
- Unique user logins and roles (i.e., admin, viewers)
- Create alerts based on metrics and send custom notifications

SCANS



SCANS on GitHub (currently private)

SCANS

Simple Containerised Analysis for NMR Systems

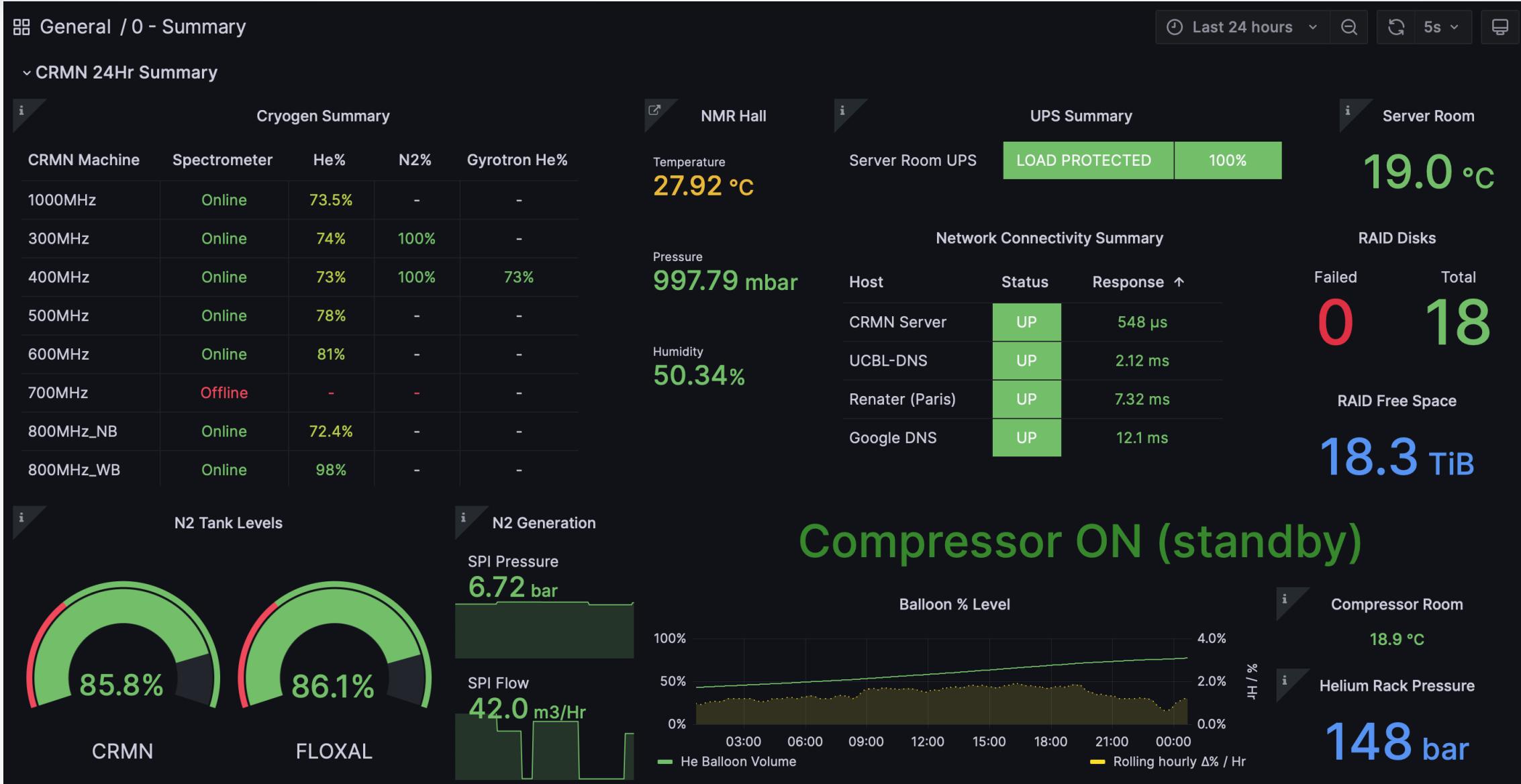
SCANS brings together multiple open-source tools and custom Python scripts to provide basic dashboard monitoring, with easily customizable analysis, data visualisations, and alert management. It was created with NMR laboratories in mind, however, data from any system can be incorporated or be the sole focus. Provided examples include monitoring of auto-generated NMR Spectrometer logs (Bruker/MICS), RAID-array capacity, API-retrieved data mining, non-API web-scraping (Bruker-HLMU, UPS), and monitoring of industrial hardware such as compressors (via ModBus-RTU).

Disclaimer: for the moment, SCANS is simple in its analysis and compute requirements but less so in its manual setup. You don't need to be skilled in programming - but knowledge of regex and proficiency with UNIX systems are recommended. I aim to create an automated setup tool in the future.

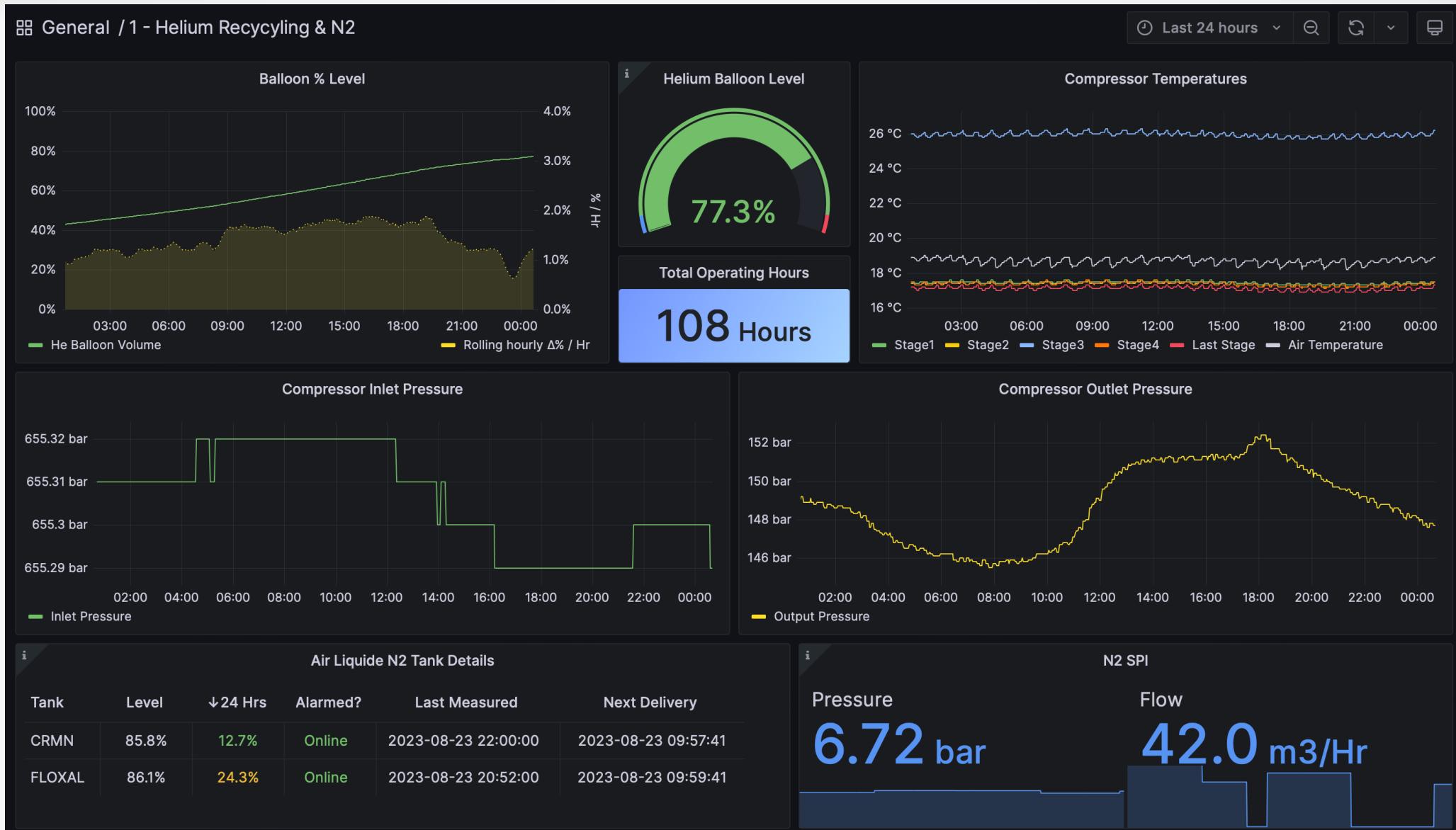
The GitHub repository for SCANS contains 132 commits across 1 branch and 0 tags. The latest commit, 81ee9f5, was made 13 hours ago. The repository is currently private.

| Commit | Author | Message | Date |
|--------------------|-----------|--|--------------|
| 81ee9f5 | jtolchard | Add UPS alert icon | 13 hours ago |
| Client-EnvSensor | | Added Client for Lab Sensor | last week |
| Client-N2_scrapers | | Added func. to check API2 for latest value | yesterday |
| Client-RAID | | Mass revision for V2 | 4 months ago |
| Client-UPS | | fix for cron | 2 weeks ago |
| Client-gyro | | Added module to read HMLUs for gyrotron | last month |
| Client-remote | | Added module for logging remotely-run commands | last month |
| Client-spec | | corrected mounted logfile name | last month |
| MICS | | add screenshots for mics setup | 2 months ago |
| Monitor | | Updated prom-long for Lab Sensor | last week |
| Network-Tester | | Added module for network analysis | last month |
| Other | | Consolidating updates | 2 days ago |
| icons | | Add UPS alert icon | 13 hours ago |
| standalonescripts | | Added standalone scripts directory | last month |
| .gitignore | | Made gitignore more selective | last month |
| Changelog | | update | last month |
| Future addons.lua | | ideas file | 2 months ago |

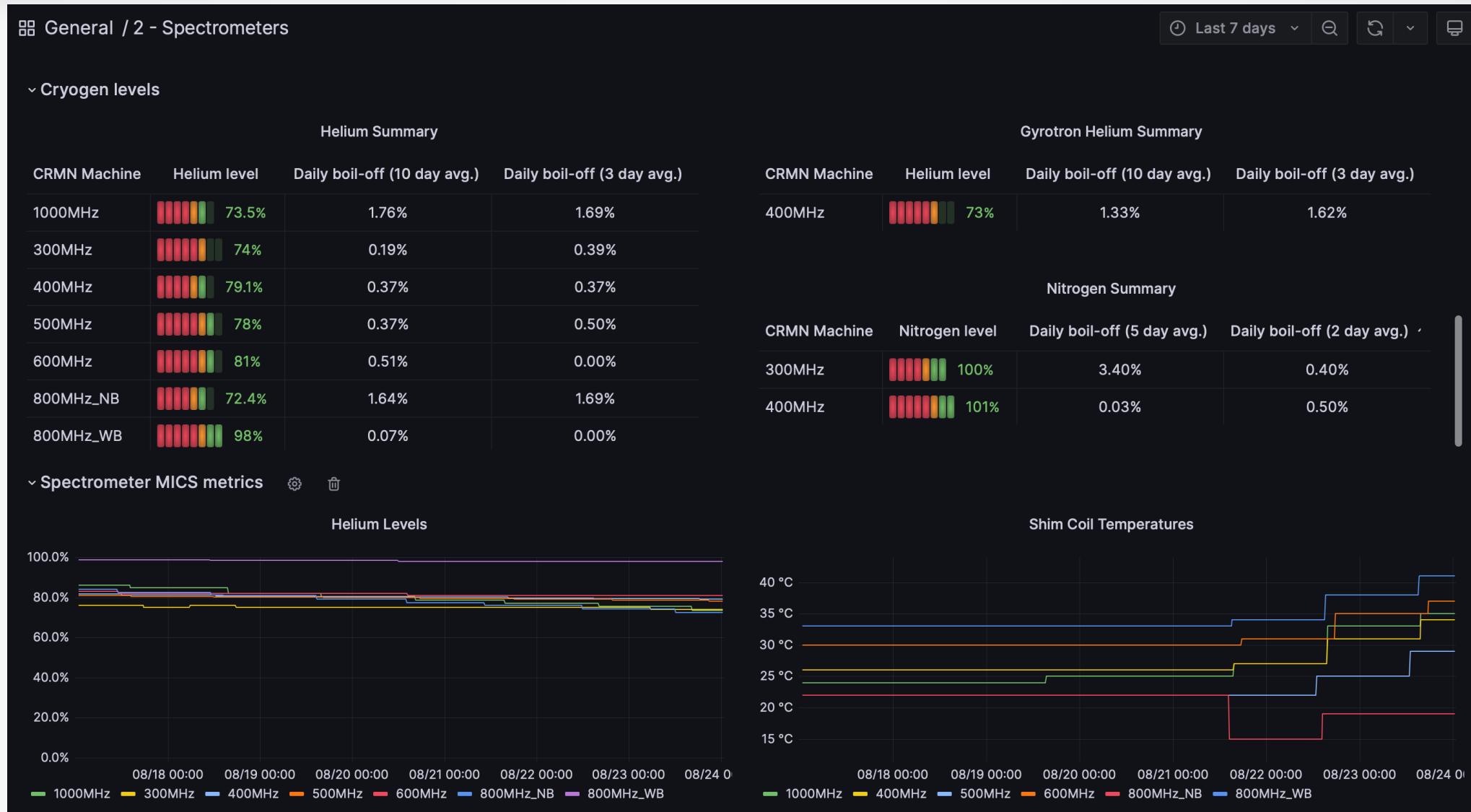
SCANS Dashboard: Summary



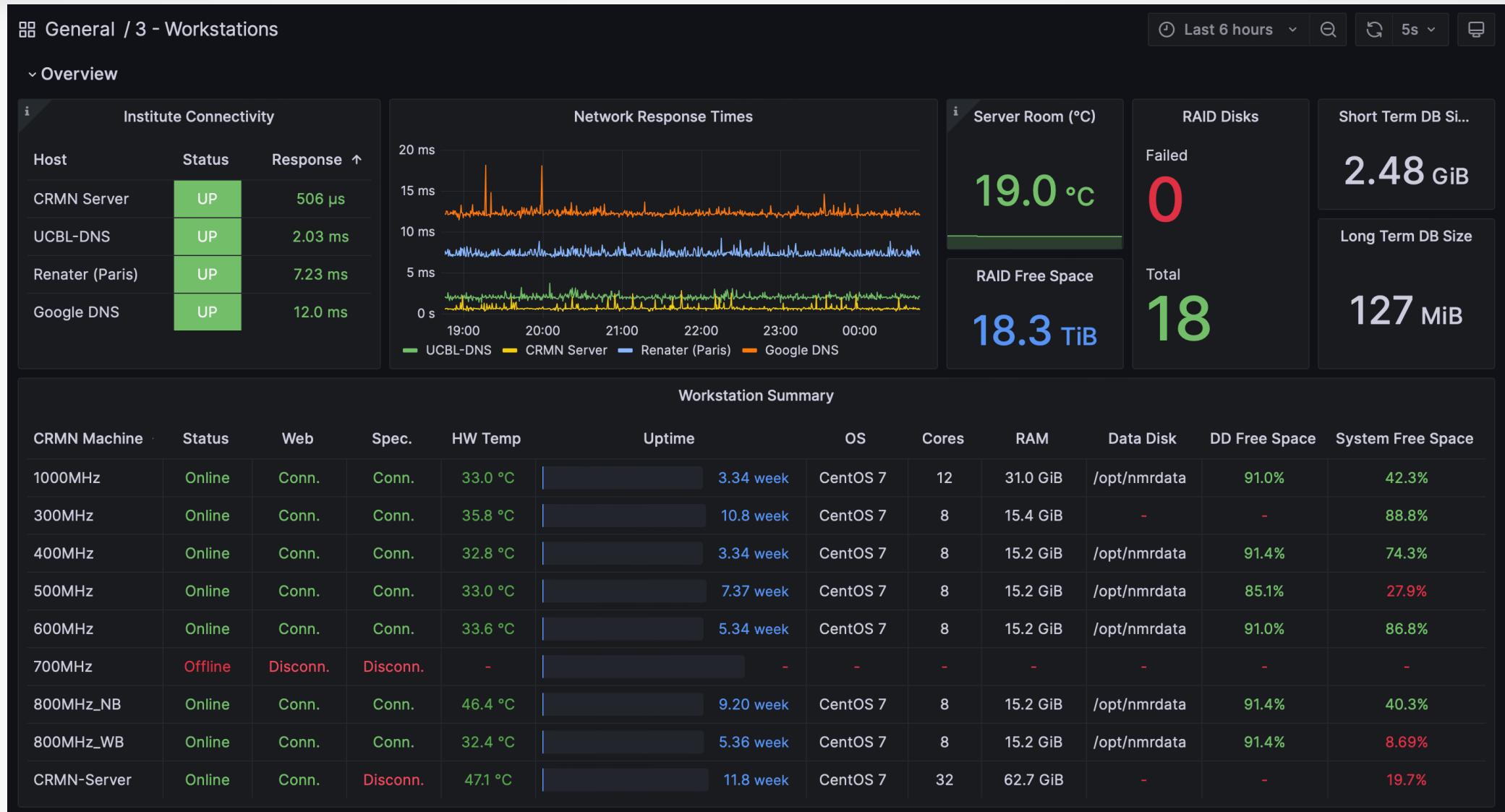
SCANS Dashboard: Cryogen metrics



SCANS Dashboard: Spectrometer metrics



SCANS Dashboard: Workstation metrics



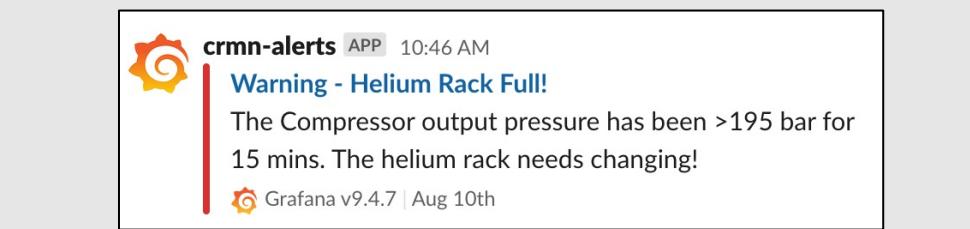
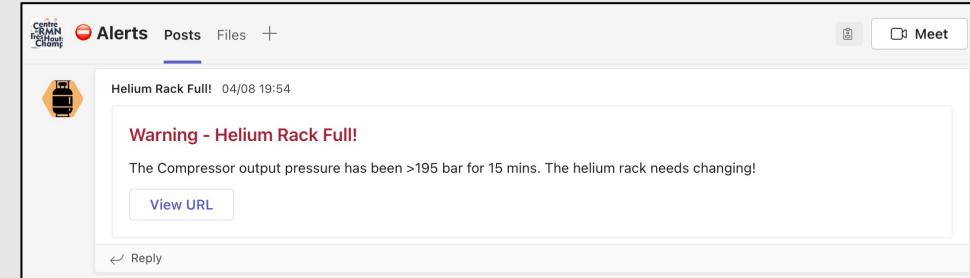
SCANS: Current Automated Alerts

- UPS Discharging
- Server room air conditioning fail ($>30^{\circ}\text{C}$)
- RAID disk fails

-
- Compressor room air conditioning fail ($>30^{\circ}\text{C}$)
 - Helium full – needs changing (>195 bar)

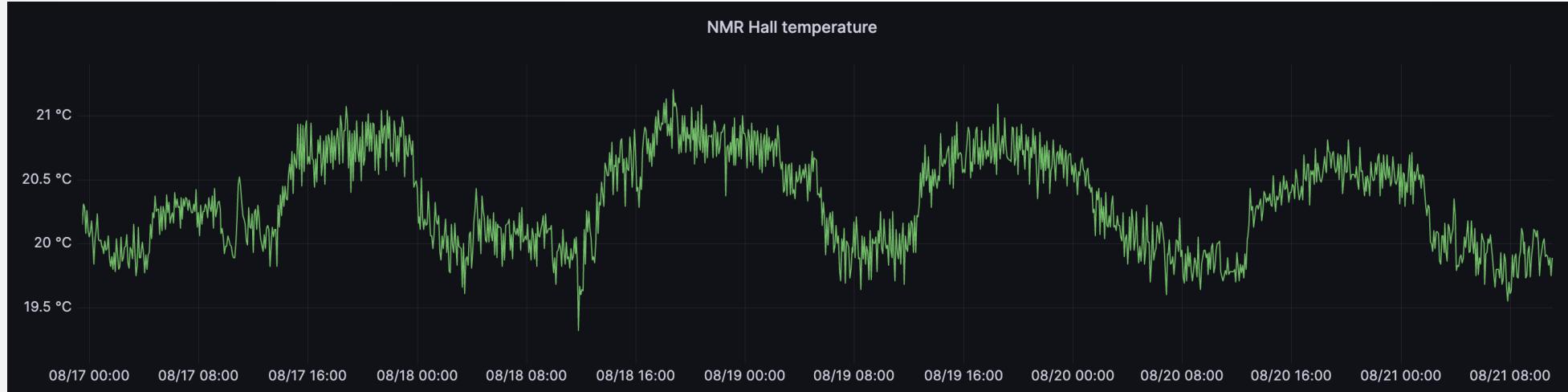
-
- FLOXAL N2 low pressure (<1 bar)
 - Air Liquide LN2 tanks, high usage (20%/hr)
 - Air Liquide LN2 tanks, low level (<33%)

Alerts currently sent to custom
#alerts Slack & Teams channels



Observations so far...

Normally, NMR hall temp is regulated between ~20-21°C)



Observations so far...

But, in a heat wave, the Air Conditioning regulation fails... and NMR Hall can reach ~30.4°C!

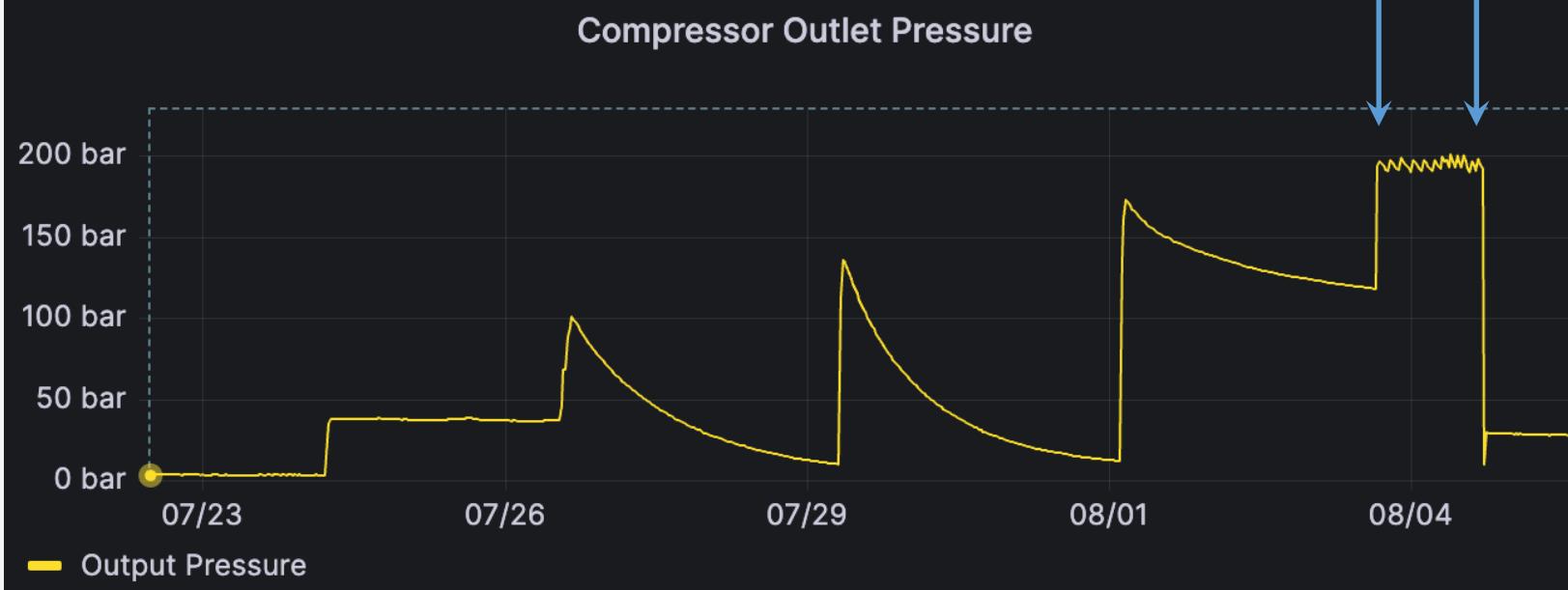


Observations so far...

Humans make mistakes...

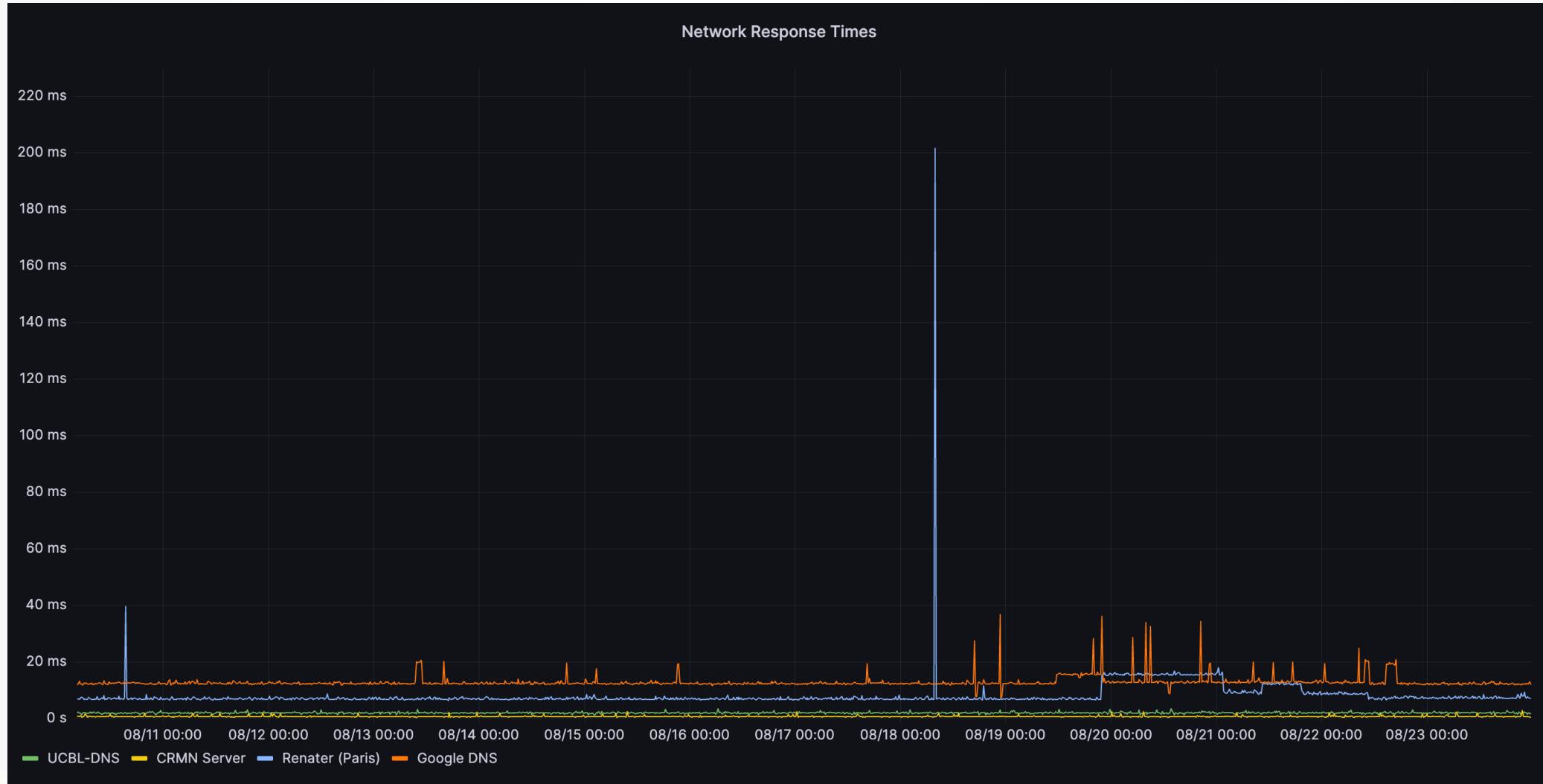
- new helium rack connected (but not opened)

26 Hrs



Observations so far...

Our Network connectivity issues seem to be resolved



Observations so far...

The Topspin data directories are mounted incorrectly on the 500 MHz and 800 MHz WB

- luckily informed user before summer experiments!

| Workstation Summary | | | | | | | | | | | | |
|---------------------|---------|-------------|-------------|---------|-----------|----------|-------|----------|--------------|---------------|-------------------|--|
| CRMN Machine | Status | Web | Spec. | HW Temp | Uptime | OS | Cores | RAM | Data Disk | DD Free Space | System Free Space | |
| 1000MHz | Online | Conn. | Conn. | 32.9 °C | 3.34 week | CentOS 7 | 12 | 31.0 GiB | /opt/nmrdata | 91.0% | 42.3% | |
| 300MHz | Online | Conn. | Conn. | 35.6 °C | 10.8 week | CentOS 7 | 8 | 15.4 GiB | - | - | 88.8% | |
| 400MHz | Online | Conn. | Conn. | 33.2 °C | 3.34 week | CentOS 7 | 8 | 15.2 GiB | /opt/nmrdata | 91.4% | 74.3% | |
| 500MHz | Online | Conn. | Conn. | 33.4 °C | 7.36 week | CentOS 7 | 8 | 15.2 GiB | /opt/nmrdata | 85.1% | 27.9% | |
| 600MHz | Online | Conn. | Conn. | 33.6 °C | 5.33 week | CentOS 7 | 8 | 15.2 GiB | /opt/nmrdata | 91.0% | 86.8% | |
| 700MHz | Offline | Disconnect. | Disconnect. | - | - | - | - | - | - | - | - | |
| 800MHz_NB | Online | Conn. | Conn. | 46.4 °C | 9.19 week | CentOS 7 | 8 | 15.2 GiB | /opt/nmrdata | 91.4% | 40.3% | |
| 800MHz_WB | Online | Conn. | Conn. | 32.8 °C | 5.36 week | CentOS 7 | 8 | 15.2 GiB | /opt/nmrdata | 91.4% | 8.69% | |
| CRMN-Server | Online | Conn. | Disconnect. | 46.7 °C | 11.8 week | CentOS 7 | 32 | 62.7 GiB | - | - | 19.8% | |