

# SCANS

## An open-source modular system for laboratory monitoring, dashboards, and alerts

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### NMR laboratories are complex environments!

Platform operations rely on the consistent performance of various elements, such as environmental controls (air conditioning, fridge-freezers, glove-boxes), spectrometer hardware (consoles, magnets, gyrotrons, cryo-platforms), IT systems (resource availability), and general infrastructure (battery backups, compressors, chillers, pumps).

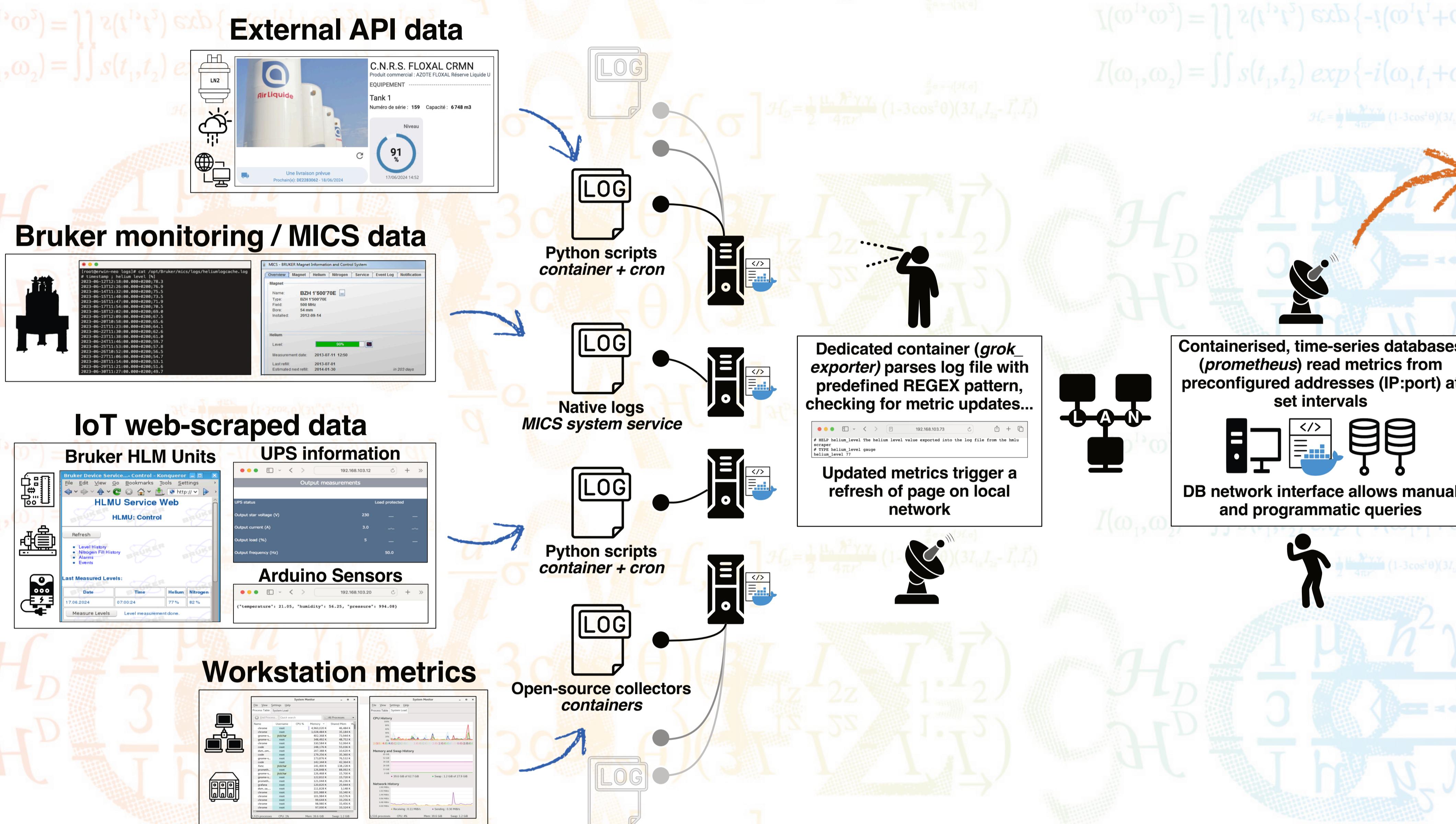
Many typical problems can often be foreseen, or their damage minimised, by close monitoring of the relevant system metrics. However, academic laboratories typically contain a combination of off-the-shelf and niche scientific, commercial, and custom-built equipment with no consistent communication standards, logging formats, or monitoring tools.

General laboratory-monitoring tools do exist, but they can be expensive and lack comprehensive hardware coverage. Worse still, monitoring of NMR hardware in particular is overly reliant on direct human interactions and automated warnings via analogue telephone.

By using open-source tools originally developed for systems monitoring, in combination with the programmatic standardization of hardware log files, we propose a versatile and cost-effective monitoring solution suitable for an academic setting with customizable dashboarding and alerts.



### Simple Containerised Analysis for NMR Systems



### Simple setup and minimal system requirements

SCANS uses containerization to simplify the installation and configuration of all necessary components for monitoring. Containers can be thought of as small virtual machines with the minimal number of packages needed to support a specific microservice (such as a script, tool, database, or server).



Containers are managed and downloaded by a central engine called Docker, which is free and simple to install on Linux, Mac, and Windows (64-bit, via WSL). Once installed, the configuration files provided with SCANS can be used to quickly set up and configure the relevant modules.



### No log files or network-connection? No problem!

SCANS was initially built to collect information from the pre-existing log files created by Bruker NMR systems.

However, a number of important elements only had web- or MODBUS-accessible metrics, with no log files from which to scrape information. The solution? We created our own log files! Containers with custom Python scripts were developed to routinely crawl web pages or remote devices for data, and generate log files in a format that best suited our needs. Examples include metrics concerning our Bauer compressor and Helium recovery system, as well as parameters from our uninterruptible power supply and -80 °C freezers.

Another issue was that not all hardware was freely network-connected. The solution? We developed our own network-connected interfaces and sensors using Arduinos. By publishing metrics on the network in parsable JSON output, custom log files can be generated, and the metrics recorded.



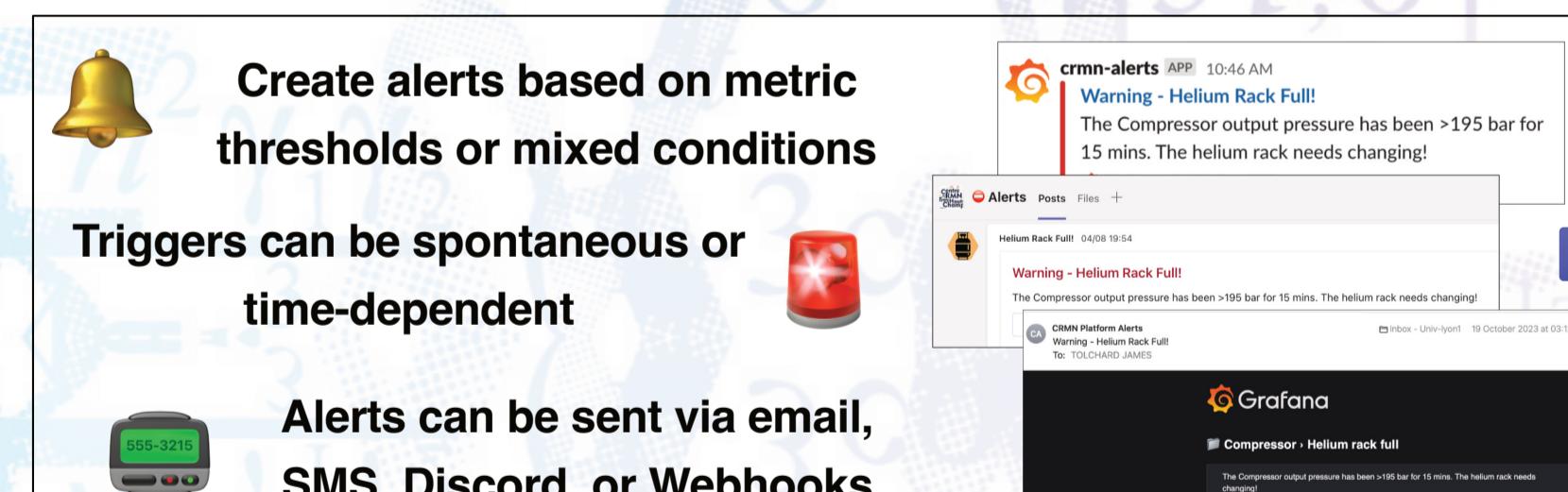
The network-connected Arduinos reporting environmental conditions (top-left) and freezer alarm states (top-right), and their corresponding JSON outputs which can be routinely scraped and made accessible in SCANS for reporting, plots, and alarms (bottom). Arduino code and 3D-printed cases can be found in the SCANS GitHub repository.

### Grafana analytics & visualization

#### Online dashboarding



### Alerts & notifications



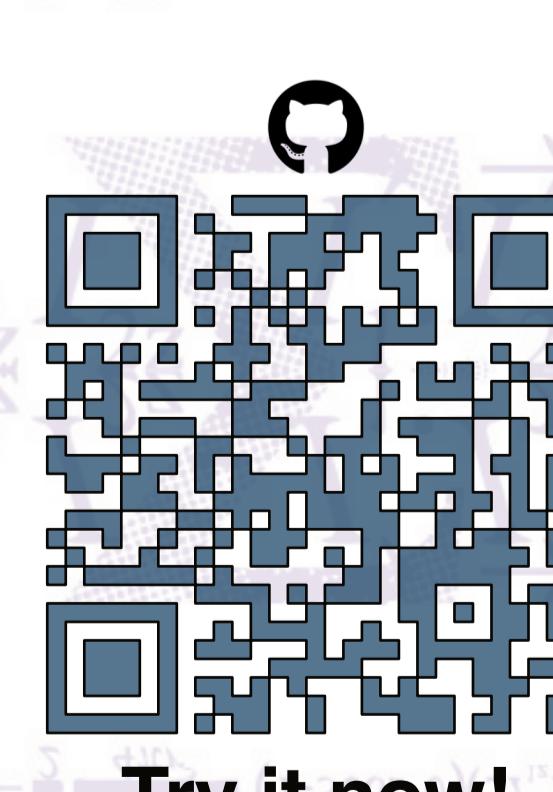
### Future Development

The CRMN NMR platform in Lyon has been using SCANS successfully for the past 11 months. During this time, it has identified a number of hardware issues and has been invaluable in optimizing our recent Helium recovery system. This version of SCANS is currently available as a GitHub repository for public use.

However, there are a number of elements marked for improvement:

Firstly, in a multi-spectrometer setting, the monitoring and logging system relies on multiple software installations (of Docker and at least one container). While functional, this could be simplified by having a single installation, with all logs retrieved over a local network. A 'remote' module is already working to accommodate older unsupported hardware, and this functionality will soon be added to help collect spectrometer metrics.

Secondly, having a singular installation will also make the overall configuration simpler (i.e., defining spectrometer connection details and default ports), however a GUI would be optimal, and is therefore planned to aid in configuration and use by non-expert users.



Try it now!

