AGI 4: Hacky Hour II (joint session AGI/SOE/AKjDPG)

In this new format, introduced by AGI and jDPG, tools are presented that can be helpful in your everyday scientific work. Whenever possible a hands-on part will be offered where the tool can be used directly preferably on your own laptop. Furthermore there will be a discussion of the tool where e.g. aspects of compatibility and extensibility can be addressed.

If installation of software is necessary in advance instructions on this and further information in general can be found at https://hacky-hour.dpg-physik.de

Time: Wednesday 15:00–18:00 Location: MAR 0.011

AGI 4.1 Wed 15:00 MAR 0.011

Controlling experiments and recording FAIR data with NOMAD CAMELS — •Alexander D. Fuchs[1,2], Johannes A. F. Lehmeyer[1,2], Heiko B. Weber[1], and Michael Krieger[1] — [1]Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany. — [2]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany

NOMAD CAMELS (Configurable Application for Measurements, Experiments and Laboratory Systems) [1] is an open-source measurement software that records FAIR and fully self-describing measurement data. It enables the definition of measurement protocols via a graphical user interface without requiring programming knowledge or deeper understanding of instrument communication. Coming from the field of experimental physics, CAMELS provides the flexibility of controlling a large variety of measurement instruments in frequently changing experimental setups. The user-defined measurement protocols are translated into stand-alone executable Python code, providing full transparency of the actual measurement sequences.
This Hacky Hour contribution starts with a brief overview of CAMELS followed by a hands-on session on setting up CAMELS and performing measurements (to follow bring your own laptop if possible).
[1] https://fau-lap.github.io/NOMAD-CAMELS

AGI 4.2 Wed 15:45 MAR 0.011

Streamlining Data Management in Laser Plasma Experiments with Python-Flask WebApps — •Kristin Tippey, Hans-Peter Schlenvoigt, and Thomas Kluge — Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstraße 400, 01328 Dresden, Germany

In the complex field of laser plasma experiments, managing data efficiently and effectively is crucial. The goal of our team is to establish a standardized, efficient, and user-friendly system that adheres to FAIR principles, with ambitions to enhance the research and analysis capabilities of the teams at Helmholtz Zentrum Dresden-Rossendorf (HZDR). We are creating an integrated ecosystem comprising of a set of Python-Flask WebApps, each playing a role in the process of logging and managing data in these specialized experiments. The current collection of applications include features for the direct capture of manually entered parameters, software trigger and ID distribution, generic data collection, and experiment actuator logging. Additionally, scripts are being devised to collect metadata from a selection of simulation input styles for upload to SciCat for eventual cross-referencing of simulations with experiments. The effective cataloging of data and metadata not only benefits our machine learning team but also promises to enrich experimental analysis and decision-making processes. Additionally, our software can serve as a reference model for similar systems or be adapted for deployment in other environments, extending and augmenting existing systems as appropriate.

15 min. break

AGI 4.3 Wed 16:30 MAR 0.011

elabFTW as one building block of our FAIR data exchange — •Sebastian T. Weber, Eva Walther, Martin Aeschlimann, Bärbel Rethfeld, and Georg von Freymann — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau

The basis of a FAIR data management is a well-described and detailed documentation of every single step of the experiment and data analysis. In recent decades, however, the focus has shifted from analog measuring instruments and analytical calculations to computer-based experiments and simulations. This has lead to a large increase in the numbers of measurements and observed quantities and therefore in the amount of data generated.

We use electronic lab notebooks (ELNs) to store, index, search and retrieve a large amount of entries within our collaborative research center CCR/TRR173 Spin+X. Here, it is particularly challenging to exchange data between scientists with different background and location. In this presentation, we introduce our ELN 'elabFTW' and give insight into our journey of establishing a joint electronic lab notebook as well as harmonizing the exchanged meta(data) to foster collaboration within our research center. We report on our experiences in the daily work of the scientists and our progress of a new infrastructure project.

AGI 4.4 Wed 17:00 MAR 0.011

Computational Notebook as a Modern Multitool for Scientists — •Kirill Vasin — Augsburg University, Augsburg, Germany

Modern computational notebooks, stemming from the 1981 Literate programming concept, are powerful tools like Mathematica, Maple, and Jupyter Notebook. Yet, popular solutions often lack traditional math input support, focusing on specific fields (business analytics, engineering or solely computer algebra) or not being open/freeware.

For physicists, OriginPro, PowerPoint, and paper are preferred, as notebook interfaces are challenging to use efficiently. To address this, we developed WLJS Notebook [https://jerryi.github.io/wljs-docs/], a scientist-designed system based on Wolfram Language. It's open, friendly for mathematicians, allows mixing code and mathematical equations, figures preparation and covers all basic tasks experimentalists need like processing raw data and interactive fitting. With built-in support for various cell types, it facilitates data-driven interactive slides, eliminating export needs of graphs to .png files and syncing data to it. Markdown and plain HTML are used as a default languages for notes and slides.

Accessibility is ensured through export to .html or .pdf. WLJS Notebook runs locally, without internet dependency, and is free.

AGI 4.5 Wed 17:30 MAR 0.011

snip: user-centered lab book — •Markus Osterhoff, Sebastian Mohr und Sarah Köster — Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Conducting and steering complex experiments is a highly creative process, requiring not just the alignment, sample treatment, and preliminary analysis, but also real-time discussions among researchers. In the realm of traditional hand-crafted log books, there was significant freedom to combine printouts with annotations and sketches, mirroring the progress and decisions of the experiment. However, with the advent of electronic log books, the creativity in free note-keeping has been largely disregarded, with an overemphasis on formalities consuming more time. Moreover, important machine parameters, like motor positions and images from detectors and microscopes, are not easily accessible or referenced, even in facility-developed log books.

We propose "snip," a digital user-centered lab book that combines hand-crafted entries with computer-generated content. This system not only supports standard measurements but puts creative research at the forefront. Through external software (control software, detector and microscope computers, etc.), standardized "snippets" representing the experiment are created and sent. Researchers can curate these snippets, adding annotations and using a pen for quick documentation, sketching, and highlighting. The web-based software facilitates collaborative work, allowing experts worldwide to work on the document simultaneously and discuss their ideas in real-time.

The "snippets" carry essential information as metadata, like motor positions or images. Before being "glued" into the book, users can adjust the actual "view" (size, ROI, etc.), and then annotate with pen entry. This maintains the "analogue mode of operation" to a large degree, but instead of printouts, "true digital copies" are used. Furthermore,

an API provides definable interfaces for third-party software (control, analysis, simulation) to submit digital versions of the traditional paper snippets, including system state printouts or graphics.

In this way, snips are not automatically or strictly chronologically added to the lab book. Instead, users creatively curate them according to the ongoing discussion, enriching the machine-readable information with sketches, highlights, and ad hoc texts. This approach not only preserves but enhances the creative and collaborative aspects of experimental research, integrating the flexibility of digital technology with the intuitive, hands-on approach of traditional scientific exploration.