Working Group "Young DPG"
Arbeitskreis junge DPG (AKjDPG)

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Overview of Invited Talks and Sessions

(Lecture hall MAR 0.002)

Sessions

AKjDPG 1.1–1.1	Mon	14:00–15:00	MAR 0.002	**Global challenges and how we can overcome them**
AKjDPG 2.1–2.3	Mon	15:00–16:30	PTB HS HvHB	**Transformation Processes in Scientific Publishing – A Discussion (joint session AGI/SOE/AKjDPG)**
AKjDPG 3.1–3.6	Wed	9:30–12:25	MAR 0.011	**Hacky Hour I (joint session AGI/SOE/AKjDPG)**
AKjDPG 4.1–4.5	Wed	15:00–18:00	MAR 0.011	**Hacky Hour II (joint session AGI/SOE/AKjDPG)**

AKjDPG 1: Global challenges and how we can overcome them

Time: Monday 14:00–15:00 Location: MAR 0.002

Discussion AKjDPG 1.1 Mon 14:00 MAR 0.002
Global challenges and how we can overcome them jDPG and TPSA — •Zoé Abraham[1], Cyrus Pan Walther[3,4], and Thi Dieu Hien Van[2] — [1]jDPG — [2]National Yang Ming Chiao Tung University Taiwan — [3]TU Dortmund — [4]IAPS

Climate change, health and security are just three of the many global challenges we face as a society today. As physicists, we are doing our part to help solve some of these problems. It is important that not every country finds solutions on its own and is keeping them to themselves, but that there is open communication and progress is shared. We want to discuss how the application of physics can help to develop new technologies an innovations that contribute to overcoming global challenges and how a cooperation between different countries and cultures can look like. As these global challenges mainly concern young people, a young person from Taiwan will be invited as well as a person from Germany. The panel discussion will be moderated by Zoé Abraham from jDPG.

AKjDPG 2: Transformation Processes in Scientific Publishing – A Discussion (joint session AGI/SOE/AKjDPG)

Time: Monday 15:00–16:30 Location: PTB HS HvHB

Invited Talk AKjDPG 2.1 Mon 15:00 PTB HS HvHB
The future of scientific publishing, for and by scientists — •Roderich Moessner — Deutsche Physikalische Gesellschaft — MPIPKS Dresden

The landscape of scientific publishing has been very dynamic in recent years, in large part driven by a desire to transition into open access publication formats. This has raised, or refocused attention on, a number of broader issues concerning how we as scientists would like to interact with each other, and with the outside world.

In a position paper on the subject, the DPG has attempted to take stock of where we stand, what the issues are, and what the options for a way forward may be. This talk aims to introduce and give an overview over what we believe are the central issues from the point of view of practising scientists.

Invited Talk AKjDPG 2.2 Mon 15:15 PTB HS HvHB
On the status of Open Access publishing in Germany — •Gerard Meijer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In the framework of the DEAL-project, the scientific community in Germany is pursuing the goal of transforming the academic publishing system from a subscription-based system, in which publications are locked behind a paywall, to a system where there is Open Access to scientific publications. OA increases the visibility of the published research, which is of direct benefit to the authors who want their research findings to be known and acknowledged. In OA publishing the copyrights remain where these belong, namely with the authors. Openly accessible publications can be read, reviewed and used more widely by other researchers. This increases the quality of research and accelerates scientific progress. OA makes scientific knowledge more widely available outside of the scientific community and lowers the threshold for various transfer activities. This increases the social effectiveness of (publicly funded) research.

In spite of all these advantages, which are apart from the cost-savings for Germany as a whole, the DEAL-project is viewed upon critically by many. In this short entrance statement, I will therefore focus on the factual achievements.

Discussion AKjDPG 2.3 Mon 15:30 PTB HS HvHB
The Future of Our Publication System — •Uwe Kahlert[1], Vivienne Leidel[2], Roderich Moessner[3], and Gerard Meijer[4] — [1]RWTH Aachen University — [2]DPG — [3]DPG, MPIKS Dresden — [4]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Over the last two decades discussions continued on how the scientific publication system should and could be transformed to better reflect the demands of scientists. The national DEAL initiative negotiated agreements with three major publishers to initially advance this transformation at a national level. After a short introduction on these topics by representatives of the DPG and DEAL in the previous talks we want to discuss with them what changes this means for scientists and how the transformation can or should continue.

AKjDPG 3: Hacky Hour I (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 9:30–12:25 Location: MAR 0.011

AKjDPG 3.1 Wed 9:30 MAR 0.011
Get the most out of your data: Interactive Visualisation with Python and Plotly — •Christian Faber — Forschungszentrum Jülich, Jülich, Germany

Scientists have always been the experts for data. Analysing and drawing conclusions from them is our daily business, and the amount of data that scientists are confronted with is growing rapidly as time passes and computing resources increase. The challenge is to quickly deal with individual data structures for which there is usually no off-the-shelf solution. In this talk, I will tell you how you can create visualisations tailored to your data. I will show, how you can access your data interactively and thus gain maximum insight from it. The graphics are created using Python and the *pyplot* and *dash* libraries to achieve maximum customisability. The entire process is demonstrated using a sequence mutation example from biophysics, but the methods can be applied to any field involving large amounts of data.

AKjDPG 3.2 Wed 10:00 MAR 0.011
Blender for scientific figures and animations — •Timo Doerries — Institute of Physics & Astronomy, University of Potsdam, 14476 Potsdam, Germany

Blender is a free open source 3D tool. It can be used to produce static figures for publications [1,2]. In addition to a graphical user interface it can be completely controlled using simple Python syntax. This allows creating complex animations, that can be used to illustrate simulations. I will show how to set up a simple ray-tracing image and

animate a simulation from the field of statistical mechanics using the python interface.

[1] Doerries, Chechkin & Metzler, J. R. Soc. Interface.19 (2022)
[2] Doerries, Metzler & Chechkin, New J. Phys. 25 (2023)

AKjDPG 3.3 Wed 10:30 MAR 0.011

MicMag2, an atomistic and micromagnetic simulator python package — •Thomas Brian Winkler[1], Kai Litzius[2], Hans Fangohr[3], and Mathias Kläui[1] — [1]Johannes Gutenberg-Universität Mainz 55099 Mainz — [2]Universität Augsburg, 86159 Augsburg — [3]Max Planck Institute for the Structure and Dynamics of Matter Hamburg, 22761 Hamburg

Micromagnetic simulators are one core driver of spintronic research nowadays. We present MicMag2 [1], a combined micromagnetic and atomistic simulator which can be used within a python or jupyter framework. GPU acceleration and modular program architecture allow for fast data acquisition and flexibility in implementing custom modules. In this session we will introduce the functionalities of MicMag2, advanced and less common modules, and how data analysis can be easily transferred to numpy-based [2] code or to the ubermag framework [3]. The presentation will include an introduction into the basics of micromagnetism and a tutorial on the practical use of the software. [1] https://github.com/WinklerTB/MicMag2 [2] Harris, C.R., Millman, K.J., van der Walt, S.J. et al., Nature 585, 357*362 (2020) [3] M. Beg, M. Lang and H. Fangohr, IEEE Transactions on Magnetics, vol. 58, no. 2, pp. 1-5, Feb. 2022, Art no. 7300205

AKjDPG 3.4 Wed 11:00 MAR 0.011

Quantum Many Body Simulations with TeNPy — •Johannes Hauschild — Technical University Munich, Germany

Matrix product state (MPS) based algorithms like the density matrix renormalization group (DMRG) are established as *the* state-of-the-art method for simulations of quantum many body systems in 1D, for example Heisenberg and Hubbard type models. In fact, MPS are so successfull that they are routinely used for 2D systems as well, by mapping thin long cylinder geometries to 1D. Generalizations of MPS to natively 2D tensor network states in the form of PEPS or isoTNS provide an alternative route for competitive results, especially for cases where quantum monte carlo methods suffer from the sign problem.

I will present version 1.0 of TeNPy, the "Tensor Network Python" package that I started developing half a decade ago. The major goal has been to make MPS and tensor network simulations accessible not only to experts of the field but also new users, by excellent documentation, and balancing speed of the code with flexibility to define new models and algorithms. Indeed, TeNPy has been accepted well by the community with over 250 papers acknowledging its use and code contributions from various groups. After a (very) brief introduction to the main ideas behind the algorithms, I will show small examples for typical use cases of TeNPy. I will further discuss our ongoing efforts and first benchmarks to adapt TeNPy and the implemented algorithms to GPU-based calculations, and how we plan to incorporate the conservation of non-abelian symmetries.

15 min. break

AKjDPG 3.5 Wed 11:45 MAR 0.011

FAILS (Fancy automated internet lecture system) — •Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

In theoretical physics, the conventional lecture with chalk by slowly exploring the physical formulas is still one, if not the best method. However modern expectations of lectures include electronic scripts for students, interactive questions for student engagement, and hybrid audio/video transmission.

FAILS (Fancy Automated Internet Lecture System) is developed to meet this demand. The open source software was developed driven by the author's need to have electronic chalk on multiple projectors, interactive quizzes, chat, and also audio/video transmission in one software for lectures in theoretical physics, here at TU Berlin. All features are highly automated and designed to reduce the distraction of the lecturer. After initially being used in our institute it is now university-wide deployed in our moodle learning management system ISIS with support from innoCampus. This talk gives a short hands-on demonstration of the abilities of the FAILS software (cf. https://github.com/fails-components/compositions and https://www.youtube.com/@fails-components).

AKjDPG 3.6 Wed 12:05 MAR 0.011

Hacky teaching — •Yoav G. Pollack[1,2], Anas Hussin[1], Jaskaran Singh[1], and Komal Bhattacharyya[1] — [1]University of Göttingen, Göttingen, Germany. — [2]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Göttingen, Germany.

I examine hackathons, imported from the world of software startups, as a motivating teaching method. In December 2023, a 2-day hackathon was held for the CYTAC Research Training Group in the University of Göttingen, on the topic of simulating cytoskeleton with the Cytosim software package[by Nédélec Group]. The aims of this venture were 1) to promote initiation of collaborations by students from different research groups spanning several disciplines, 2) to encourage experiment-oriented students to do computational work, 3) to encourage theory-oriented students to consider the biological context of their theoretical research, 4) to make learning fun. I will report on the outcomes of this hackathon that managed to attract students from diverse computational backgrounds and scientific backgrounds and showcase selected proof-of-concept projects from the teams.

AKjDPG 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.

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

AKjDPG 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

AKjDPG 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

AKjDPG 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.

AKjDPG 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.

AKjDPG 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.