SOE 13: 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

SOE 13.1 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.

SOE 13.2 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)

SOE 13.3 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

SOE 13.4 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

SOE 13.5 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).

SOE 13.6 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.