AKjDPG 6: Hacky Hour

Time: Friday 9:30–12:30 Location: HSZ 105

Invited Talk AKjDPG 6.1 Fri 9:30 HSZ 105

Physicist in IT: Physics in Advent — •André Wobst — wobsta GmbH, Unterschleißheim

For more than 17 years I am working as a service provider in planning, realization and administration of physics-related IT projects. Here I present one of the projects, namely a physics Advent calendar. The technology stack is rather common and efficient: Python, Flask, PostgreSQL to name just the most important building blocks. The load of such a project (more than 43,000 users in 2019, all within a few weeks and with high daily return rate) is operated on moderate infrastructure by taking into account efficiency right from the start. I overview challenges that arise during implementation and operation and show some web analytics, monitoring data and report on attacks. I will also discuss a few pitfalls like avoiding backpressure (a term adopted from fluid dynamics to IT).

AKjDPG 6.2 Fri 10:00 HSZ 105

Reproducible workflows for reproducible science (with Snakemake) — •Johannes Hampp — Center for international Development and Environmental Research, Justus Liebig University Giessen

Daily scientific tasks with research data from experiments or simulations often imply repetitively applying the same analysis steps. Be it with R, Python or other programming languages, analysis workflows too often followed by hand. Executing analysis steps manually be the obvious approach, but is tedious and prone to human error. In this talk I introduce you to Snakemake, an open source solution for managing your workflows. Snakemake allows for well-defined workflows, with steps executed automatically in the correct and necessary order. It decreases the amount of non-scientific work spent in repetetive workflows and reduces unecessary errors. Since workflows are defined in a simple and human-readable format, using Snakemake helps to document your analysis. It increases reproducibility of research and lastly the FAIRness of research data.

In short: Snakemake makes your life a lot more fun.

AKjDPG 6.3 Fri 10:15 HSZ 105

How to Optimize your Productivity using Tiling: Terminal Multiplexing with `tmux` and Window Managing with `i3` — •Mario Udo Gaimann — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Germany

In this talk I will introduce you to two useful tools that can improve your workflow. In essence, they both offer a keyboard-controlled management of your workspaces and terminals which may – with some practise – boost your efficiency.
Firstly, I will introduce you to the terminal multiplexer `tmux`, a versatile tool to enhance your command line productivity. You will learn how to create, detach and attach `tmux` sessions and how to split your terminal into multiple panes and windows.
Secondly, we will have a look at the window manager `i3`, a desktop environment that allows you to optimize your workspace organization. Here you will learn how to open terminals and applications in an `i3` environment, create and split windows, change container layouts, and create new workspaces.

AKjDPG 6.4 Fri 10:30 HSZ 105

Better than histograms: Kernel density estimators and why you should use them — Alexandra Völkel[1] and •Simeon Völkel[2] — [1]Universität Bayreuth, Experimentalphysik VIII, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Universität Bayreuth, Experimentalphysik V, Universitätsstraße 30, 95447 Bayreuth, Germany

We show why everyone who has ever made a histogram should learn about kernel density estimation.

Histograms, as commonly used for estimating probability densities, are far from being optimal. In addition, they require two parameters, bin width and position, to be chosen.

Kernel density estimatiors are an easy to use drop-in replacement for virtually all histograms you ever wanted to draw. They combine superior mathematical properties with an at least as intuitive presentation. Their bandwidth, being the only parameter, can be chosen in an optimal sense automatically and adaptively.

Regarding practical application, we discuss their usage in gnuplot and python.

AKjDPG 6.5 Fri 10:45 HSZ 105

LeMonADE - A Lattice Monte Carlo Library — •Martin Wengenmayr[1,2], Toni Müller[1,2], and Ron Dockhorn[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]TU Dresden, Germany

LeMonADE is a **L**attice-based **e**xtensible **Mon**te-Carlo **A**lgorithm and **D**evelopment **E**nvironment library developed in the group "Theoretical Polymer Physics" of the Leibniz Institute for Polymer Research. It provides a C++ template meta programming interface for Monte Carlo simulations specialized for the Bond Fluctuation Model to investigate polymeric materials. Based on compile-time generated code, the framework provides containers for coordinates, topologies, and various types of metadata, also basic evaluation tools and convenience methods for I/O file handling using a human readable, compressed file format. LeMonADE has been used to simulate a wide variety of coarse-grained polymer systems under excluded volume conditions, selective solvents, nearest neighbor interactions, polymerization processes, external potentials, and even more. In addition to the CPU-based library some GPU accelerated modules are available benefiting from multiprocessor architectures. Furthermore, a visualization tool is offered as well. The project is hosted under GPL on github [https://github.com/LeMonADE-project] with a continuous integration framework running a large set of unit tests. The library has already been used for a wide range of research topics and for several publications in the field of theoretical polymer science.

AKjDPG 6.6 Fri 11:00 HSZ 105

`pyscal`: A python module for structural analysis of atomic environments — •Sarath Menon, Grisell Díaz Leines, and Jutta Rogal — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

Structural characterisation of local atomic environments is essential to provide insight into atomistic mechanisms of transformations between crystalline and liquid phases, or the formation and dynamics of extended defects that govern materials properties. The development of methods and tools to analyse the local structure constitutes a central step in the evaluation of atomistic simulation data. `pyscal` is a Python module designed for the computation of local structural order parameters during post-processing of atomistic trajectories. `pyscal` provides various approaches for structural characterisation such as Steinhardt's bond order parameters, tools for Voronoi tessellation, algorithms for clustering of atoms, and additional structural features such as radial distribution function and coordination numbers. While Python offers the advantage of flexibility and extensibility, the core code for `pyscal` is written in C++ to ensure fast and efficient calculations. `pyscal` brings together various methods for structural analysis in a single module, making it a useful tool for analysis and for applications such as feature engineering for machine learning. The source code for pyscal is available from the repository(`https://github.com/srmnitc/pyscal`) and documentation including examples are available on pyscal website(`https://pyscal.com`).

AKjDPG 6.7 Fri 11:15 HSZ 105

Scaling of Hybrid Quantum Classical Annealing — •Aditi Misra-Spieldenner[1], Peter Ken Schuhmacher[1], Xi Dai[2], Salil Bedkihal[2], and Frank K Wilhelm[1] — [1]Universität des Saarlandes — [2]University of Waterloo

In an earlier work an efficient gap-independent cooling scheme has been proposed for a quantum annealer that benefits from finite temperatures for single qubit systems based on superconducting flux qubit [1]. In our current work we extend this investigation to systems containing larger number of qubits. We simulate random annealing schedules using a well established path integral method called 'Quasi Adiabatic Propagator Path Integral' (QUAPI). We investigate different cooling methods to counter noise and heating that arise from always present longitudinal thermal noise.

[1]'Gap-independent cooling and hybrid quantum-classical annealing', L. S. Theis, Peter K. Schuhmacher, M. Marthaler, F. K. Wilhelm

AKjDPG 6.8 Fri 11:30 HSZ 105

LEED Analysis Software: LEEDCal and LEEDLab — •Roman Forker, Felix Otto, Falko Sojka, and Torsten Fritz — Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena (Germany)

Low-energy electron diffraction (LEED) can be used to measure surface lattice parameters very accurately, under the condition that the device is properly calibrated. LEEDCal provides a powerful algorithm to determine and correct systematic distortions in LEED images. Easy to operate via its graphical user interface, LEEDCal automatically generates a correction matrix upon analyzing a reference sample exhibiting a well-known surface structure. This matrix can be applied to rectify all future diffraction patterns recorded with the same LEED device. This also works in batch mode.

The results allow interpreting accurately and objectively the lattice constants and epitaxial relations when used in combination with LEEDLab, a software package that simulates LEED patterns and analyzes them quantitatively.

In our contribution, we demonstrate the functionality of the LEED analysis software packages LEEDCal and LEEDLab by means of an instructive example.

https://www.organics.uni-jena.de/en/Research.html

AKjDPG 6.9 Fri 11:45 HSZ 105

Characterizing the speed, size and shape of droplets during their flight from an ultrasonic spray coater — •Pieter Verding — Uhasselt, Hasselt, Belgium

Ultrasonic spray coating is a technology offering many new possibilities, such as depositing ultrathin homogeneous layers up to 20 nm on large scale. However, its industrial application is limited due to many process parameters which have a large impact on the quality of the coating. For this reason, measuring the droplet size, speed, and concentration during the flight from the ultrasonically generated droplet to the substrate, will give insight in how to tune the process parameters. For inkjet printing, this led to dimensionless numbers that perfectly describe the ink formulation suitable for printing. However, inkjet printing is jetting only one droplet at the time, where for ultrasonic spray coating, thousands of droplets are created at the same time, making measuring the properties of the droplets during flight a complicated task.

Three different measurement techniques (Dynamic Light Scattering, Turbidimetry and a High Speed Camera as reference) have been developed in and around an ultrasonic spray coating setup. Dynamic Light Scattering shows, after Fourier transformation, shifted peaks, representing the speed of the droplets. Further, applying Turbidimetry, it is possible to determine the size of the droplets from the speed as defined by Dynamic Light Scattering. Droplets size and speed could be measured and gave comparable results as measured with a High Speed Camera. Further, the influence of the process parameters

Discussions and Tool testing