TUT 1: Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)

Artificial intelligence (AI) has become an essential tool in modern physics, enabling new approaches to data analysis, modeling, and prediction. This hands-on tutorial provides an accessible introduction to key AI concepts, emphasizing their practical applications in physics research.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 10.03.2025, accessible via the following options:

GitHub repository:
https://github.com/RedMechanism/DPG-SKM-2025-Tutorial-AI-Fundamentals-for-Research

ZIP file download:
https://jlubox.uni-giessen.de/getlink/fiAGRzcGTiCL3GZxk8WAjom4/

Participants are encouraged to download them ahead of time.

Organized by Jan Bürger (Aachen), Janine Graser (Duisburg), Robin Msiska (Duisburg/Ghent), and Arash Rahimi-Iman (Gießen), with support from Stefan Klumpp (Göttingen) and Tim Ruhe (Dortmund).

Time: Sunday 16:00–18:15 Location: H2

Tutorial TUT 1.1 Sun 16:00 H2

Introduction — Jan Bürger[1], •Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session begins with an overview of essential AI concepts, including neural networks, training methodologies, and key distinctions between AI models. Participants will gain a foundational understanding of AI principles and how these tools can be leveraged for various research challenges.

5 min. break

Tutorial TUT 1.2 Sun 16:40 H2

Hands-On Session 1 – Function Approximation — •Jan Bürger[1], Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

In the first half of the interactive session, participants will work with Jupyter Notebooks to explore practical applications of machine learning. They will train simple neural networks to predict a mathematical function, gaining hands-on experience in tuning key parameters. Since neural networks can typically be considered universal function approximators, this concept is effectively illustrated using a one-dimensional function, making it easy to visualize and understand.

5 min. break

Tutorial TUT 1.3 Sun 17:30 H2

Hands-On Session 2 – Classification and More — Jan Bürger[1], Janine Graser[2], •Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session demonstrates how pre-trained models can simplify tasks such as classification, making them readily applicable to research. Typical examples include recognizing handwritten digits, which showcase the power of pretrained models in solving common challenges. As a preview of advanced topics, the tutorial concludes with brief examples of large language models (LLMs) and generative AI.

TUT 2: Tutorial: How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science (joint session O/TUT)

NOMAD (nomad-lab.eu) [1] is an open-source, community-driven data infrastructure, that supports automated (meta)data extraction from a wide range of simulations, including ab initio and advanced many-body calculations as well as molecular dynamics simulations. NOMAD allows users to store both standardized and custom complex simulation workflows, which not only streamlines data provenance and analysis but also facilitates the curation of AI-ready datasets. This tutorial will focus on recently developed workflow functionalities and utilities within the NOMAD infrastructure. These advances enable high-throughput interfacing with the NOMAD repository, opening improved discovery pipelines by leveraging the benefits of NOMAD's comprehensive and FAIR-compliant data management system [2].

[1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

Time: Sunday 16:00–18:00 Location: H3

Tutorial TUT 2.1 Sun 16:00 H3

FAIR-data management with the NOMAD infrastructure: Core functionalities — •Joseph F. Rudzinski — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this first part of the tutorial series, an overview of the NOMAD infrastructure will be provided. Attendees will learn how NOMAD processes raw data and stores it within a generalized data structure, and the corresponding GUI features that allow users to comfortably browse data. An example scenario will also be set up for use throughout the remainder of the tutorial series: *A researcher with a variety of data obtained within a project workflow would like to upload this data to NOMAD in order to link it to their manuscript while exposing the details of their (meta)data and retaining the scientifically relevant connections between the individual project tasks.*

Tutorial TUT 2.2 Sun 16:30 H3

Using NOMAD's API for project management — •Nathan Daelman — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this part of the tutorial series, you will learn how to interface with NOMAD programmatically using a Python module built to simplify the API (application programming interface). Functionalities for uploading data, editing metadata of uploads, creating datasets with multiple uploads, and publishing data will be covered. Attendees will use these functionalities to manage a portion of the data from the example project workflow, in particular, the subset of data that is automatically recognized and processed by one of NOMAD's existing parsers. *(For attendees without any Python experience, an alternative route to upload via the GUI will also be demonstrated!)*

Tutorial TUT 2.3 Sun 17:00 H3

Creating custom entries in NOMAD using yaml schema and ELN integration — •Andrea Albino — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this part of the tutorial series, attendees will learn how to create custom entries to store data that is not already supported by one of NOMAD's parsers. The basics of writing a schema, using NOMAD's ELN (electronic lab notebook) integration, and how to create simple plots of your data to visualize in the GUI will be covered. Attendees will then use this knowledge to manage the remainder of the data from the example project workflow, which is not automatically recognized by NOMAD.

Tutorial TUT 2.4 Sun 17:30 H3

Creating custom workflow entries in NOMAD to link multiple uploads — •Bernadette Mohr — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this last part of the tutorial series, attendees will complete the example project workflow storage by creating a custom workflow entry in NOMAD that connects all the uploaded tasks. The basics of the schema for defining custom workflows will be covered, followed by a demonstration of the straightforward creation of the required workflow file using the same workflow utility Python module as in the first part of the tutorial series. Finally, attendees will navigate NOMAD's interactive workflow graph visualizations to investigate the uploaded data, and learn how to obtain a DOI for their workflow.

TUT 3: Tutorial: Into the Third (and Fourth) Dimension: Imaging Methods for 3D Nanomagnetism (joint session MA/TUT)

Nanostructured magnetic materials have found several applications in everyday objects, such as data storage devices, sensors, and biomedical devices. When one brings these materials to the third dimension, a variety of new physics, and opportunities for applications appear. However, until recently, the vast majority of experimental investigations have primarily been focused on 2D planar geometries, as 3D systems provide a set of experimental challenges that still needs to be overcome. This tutorial seeks to provide a comprehensive overview for both experts and non-experts in the field of 3D imaging to gain a deeper understanding of the recent advances and experimental challenges connected to the investigation of 3D magnetic systems.

Organized by Claire Donnelly (MPI-CPFS, Dresden, Germany) and Simone Finizio (Paul Scherrer Institut, Villigen, Switzerland).

Time: Sunday 16:00–18:15 Location: H4

Tutorial TUT 3.1 Sun 16:00 H4

3D Magnetic Imaging: Utilizing Synchrotron X-Ray Coherence for Nanometric Resolution in Thick Samples — •Marisel Di Pietro Martinez — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2)

In recent years, there has been a growing interest from the magnetism community in expanding to three-dimensional magnetic systems - from exploring new geometries to revealing complex magnetic textures arising in micrometer-thick samples. A key aspect of this exploration is the ability to visualize the magnetization vector field at the nanoscale throughout the entire sample, made possible by the development of

3D magnetic imaging. This technique can achieve nanometric spatial resolution in micrometer-thick samples by leveraging the penetration depth and coherence of synchrotron X-rays. Furthermore, the coherence of the X-ray beam provides magnetic contrast not only in the absorption of the transmitted wave, but also in the phase. This phase contrast enables the investigation of micron-sizes magnets, even with soft X-rays, while minimizing the sample damage. In this tutorial, I will introduce how to exploit these advantages using coherence-based techniques, such as Fourier transform holography and ptychography, to perform 3D magnetic imaging. Visualizing the magnetization vector field with nanometer spatial resolution in micrometer thick samples opens the door to studying magnetic textures in higher dimensions, offering insights into fundamental physical phenomena as well as promising new applications in information storage and processing.

Tutorial TUT 3.2 Sun 16:45 H4

Nanoscale Mapping of Magnetic Textures in 3D Using Vector Field Electron Tomography — •Axel Lubk[1,2] and Daniel Wolf[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Germany

Vector field Electron Tomography (VFET) combines Electron Holography and Electron Tomography in the Transmission Electron Microscope (TEM) to reconstruct magnetic induction vector fields in 3D down to several nanometer resolution. In this tutorial we discuss the foundations of the technique, the practical workflow including pitfalls, and application to topical examples in nanomagnetism including domain walls in nanowires and skyrmion strings.

Tutorial TUT 3.3 Sun 17:30 H4

3D magnetic imaging: an experimental window to study 3D magnetization at the nanoscale — •Aurelio Hierro-Rodriguez — Department of Physics, University of Oviedo,33007, Oviedo, Spain — CINN (CSIC-University of Oviedo) , 33940, El Entrego, Spain

The synergetic confluence of technological and scientific developments in nanofabrication and characterization techniques is paving the way towards the advance in Three-Dimensional Nanomagnetism, fuelled by the richness of phenomena and technological potential of the exploitation of the magnetization vector field in their natural dimensionality: three dimensions. In this lecture, a broad picture of the importance of the topic, in the framework of the novel physics that can be explored and exploited will be given, with a brief description of the methods that allow to fabricate almost any 3D magnetic geometry with nanometer resolution. The core of the lecture will deal with the advanced magnetic imaging techniques, which are opening a window towards the characterization of the full three-dimensional magnetization vector. Specifically, X-ray based magnetic vector tomography will be described and exemplified, showing the capabilities of the technique to volume resolve the magnetization vector field in arbitrary systems with nanometer resolution. These developments in vector magnetic imaging are making possible a change in the actual paradigm on how magnetization is characterized and studied at the nanoscale, by bringing a direct experimental probe to realize experimental micromagnetism.

TUT 4: Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics (joint session O/TUT)

This tutorial is designed for students, early-career researchers, and anyone interested in the foundational principles and practical methods for simulating magnetic materials. The journey begins with an introduction to the fundamentals of spin lattice Hamiltonians and their various forms, including a detailed discussion of their derivation (Lecture 1). Next, we explore state-of-the-art techniques for extracting magnetic exchange interactions from first-principles calculations through an engaging overview (Lecture 2). The final session (Lecture 3) delves into atomistic spin-dynamics simulations using the SPIRIT code, a versatile tool compatible with both smartphones and laptops. Throughout, we will emphasize the theoretical framework underpinning these approaches. The participants will have the freedom to explore a large range of phenomena, such as domain walls, skyrmions, and their dynamics under applied currents or torques.

Time: Sunday 16:00–18:15 Location: H10

Tutorial TUT 4.1 Sun 16:00 H10

Derivation of the spin-lattice Hamiltonian: Heisenberg, beyond Heisenberg, DMI, nematic exchange — •Hiroshi Katsumoto — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52428 Jülich, Germany

Magnetization textures, such as domain walls, skyrmions, or hopfions, are very active areas of condensed matter physics. These magnetic textures are usually explained based on the Heisenberg and the relativistic Dzyaloshinskii-Moriya interaction (DMI). Comparisons with experiments have shown that, in many cases, these interactions are insufficient, and a whole range (sometimes called a zoo) of higher-order symmetric and antisymmetric interactions have been proposed. In this tutorial, based on four elemental ingredients: Coulomb interaction, indistinguishability of electrons, spin, and spin-orbit interaction (SOI), I present a framework for systematically constructing exact spin-lattice models containing all spin Hamiltonians, including higher-order terms dependent on spin quantum numbers and lattice size. Examples of spin Hamiltonians for spin-1/2 and spin-1 systems up to four lattice sites are discussed. The tutorial also explores higher-order relativistic exchange interactions derived from SOI. I consider perturbations up to the 2nd order of SOI and organize (anti)symmetric interactions. Finally, the classicalization of quantum spin relevant to magnetism in solids is discussed, culminating in a spin-lattice model that provides a theoretical framework for extracting material-dependent exchange interactions via numerical calculations and enables the modeling of magnetic textures. – DFG supports the work through SPP-2137 Skyrmionics.

Tutorial TUT 4.2 Sun 16:45 H10

Computing magnetic exchange interactions using DFT — •Manuel dos Santos Dias — Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom

Magnetic materials are an unending source of fascinating physical behaviour which have fundamental appeal but also important technological applications. In order to understand, quantify and predict the properties of magnetic materials, we need information about the magnetic exchange interactions (introduced in the preceding tutorial), which control how the different magnetic atoms interact with each other and respond to external stimuli. This tutorial will give an overview on first-principles approaches to the calculation of magnetic exchange interactions using density functional theory (DFT). First I will outline how the properties of magnetic materials can be computed with and what capabilities are offered by different DFT codes. Next I will discuss how to map DFT calculations to spin models and when such a mapping is expected to work, followed by a discussion of the two main approaches to compute magnetic exchange interactions: the infinitesimal rotation method and the spin cluster expansion. Lastly, I will explain how to obtain simple information from the computed magnetic exchange interactions, such as the magnetic ground state and the spin wave spectrum, and how to connect to atomistic spin dynamics (for instance using the Spirit code covered in the next tutorial), Monte Carlo and micromagnetic simulations.

Tutorial TUT 4.3 Sun 17:30 H10

Hands-on atomistic spin-dynamics simulations with Spirit — •Thorben Pürling[1,2] and Moritz Sallermann[1,2,3] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, D-52425 Jülich —

[2]Physics Department, RWTH-Aachen University, D-52062 Aachen — [3]University of Iceland

Atomistic spin-dynamics is a powerful, fascinating and educational simulation approach to studying the stability and dynamics of mesoscopic spin-textures such as skyrmions on the basis of atomistic spin-models. It can be used as digital twin to experiments.In this tutorial, participants will be introduced to the atomistic spin model and learn interactively how to perform atomistic spin simulations using the Spirit code [1]. We will cover common computational methods employed in atomistic spin simulations, emphasizing their practical application through the Spirit software framework [2]. The majority of the session will be dedicated to engaging exercises, where participants will work through example problems using Jupyter notebooks that interface directly with Spirit. Participants are encouraged to come with basic knowledge of Python and bring their charged laptops to fully engage in the tutorial. We provide a website [3] to keep you updated such that you arrive at the tutorial prepared for a hands-on experience.

We acknowledge funding from the ERC grant 856538 (project "3D MAGIC").

[1] Gideon P. Müller *et al.*, 10.5281/zenodo.7746551 (2024)
[2] https://spirit-code.github.io
[3] https://spirit-code.github.io/dpg-regensburg2025

TUT 5: Tutorial: Automated Worksflows (joint session MM/TUT)

Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: H15

Tutorial TUT 5.1 Sun 16:00 H15

Hands-on Tutorial: Automated Workflows and Machine Learning for Materials Science Simulations — •Jörg Neugebauer[1], Tilmann Hickel[2], and Ralf Drautz[3] — [1]MPI für Nachhaltige Materialien, Düsseldorf, Germany — [2]BAM, Berlin, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany

Machine learning techniques in physics and materials science have revolutionized simulations and experimental analysis. Using these techniques to accurately predict, for example, material properties requires the manipulation and use of vast amounts of data. Manual processing and analysis quickly become impractical and error-prone, so the availability of automated workflows is critical to their efficient, reliable, and consistent application.

In this hands-on tutorial, we provide an interactive, practical introduction to workflow management using Pyiron (www.pyiron.org). Pyiron is an integrated materials science development environment based on Python and Jupyter notebooks that can be used for a wide range of simulation tasks, including rapid prototyping, coupling with experiments, and high-performance computing. The tutorial gives a general introduction to the use of Pyiron with a focus on atomistic simulation tasks. As a practical example, all steps of the workflow for the construction of ab initio phase diagrams will be performed interactively by all participants, e.g. the generation of DFT datasets, the training and validation of machine learning potentials as well as the construction of the phase diagram.