Third NFDI Berlin-Brandenburg network meeting: AI as an enabler for science

Report of Contributions

Contribution ID: **2**   Type: **not specified**

Multi-modal Large Language Models for Sustainability Challenges: Cases in Agriculture and Biodiversity

Masahiro Ryo explores the transformative potential of multimodal large language models (LLMs) for sustainability through two concrete examples: agriculture and biodiversity conservation. He illustrates efficiency gains in agriculture using AI techniques like YOLO, GPT-4, and T-Rex models, significantly simplifying agroecosystem predictions. In biodiversity conservation, he introduces modular "virtual ecologists" performing ecological assessments without extensive coding or training data. Emphasizing a transdisciplinary co-development approach, Ryo highlights how collaborative efforts among stakeholders can enhance model reliability and relevance. He further underscores AI's potential role in mitigating human cognitive biases, enabling more objective, consistent, and informed decision-making for complex sustainability challenges.

Presenter: Prof. RYO, Masahiro (Leibniz Centre for Agricultural Landscape Research (ZALF))

Session Classification: Tool Demos

Contribution ID: **3**   Type: **not specified**

Scientific Competitions for AI-Driven Scholarly Document Processing

This presentation will focus on a number of scientific competitions (also known as shared tasks) that we've been organising under the umbrella of the NFDI project NFDI4DataScience and AI (NFDI4DS). The talk will explain how scientific competitions work and what their overarching function in research is. The presentation will describe two iterations of the shared task Field of Research Classification (FoRC), run in 2024 and 2025 as part of the Natural Scientific Language Processing (NSLP) workshop series as well as Scientific Visual Question Answering (SciVQA) and Scientific Fact-checking of Social Media Posts on Climate Change (ClimateCheck), both of which are currently ongoing under the umbrella of the workshop Scholarly Document Processing 2025, to be held in Vienna in July. The goal of the talk is to promote the shared tasks and to encourage especially students and early-stage researchers to participate in such shared tasks.

Presenter: Prof. REHM, Georg (DFKI)

Session Classification: Keynote talk 2

Contribution ID: **4**   Type: **not specified**

Closing the loop in catalysis research

The mitigation of catalyst deactivation is of paramount importance for efficient technological processes. Due to the complexity of high-performance catalysts and their slow deterioration, it is challenging to study such processes and unravel their mechanisms. Self-driving Lab (SDL) approaches based on AI methods are required to conduct the necessary long-term experiments and drive them to maximise information content. This talk will highlight recent steps taken at the FHI Berlin towards this goal.

Presenter: Dr SCHEURER, Christoph (FHI, NFDI4Cat)

Session Classification: Tool Demos

Contribution ID: **5**   Type: **not specified**

From Queries to Conversations: Expanding Access to the MaRDI Knowledge Graph with a Chatbot Interface

The MaRDI Knowledge Graph contains structured information on mathematical research items such as mathematical papers, datasets, algorithms, and software. It can be explored in multiple ways: through a wiki-based website for intuitive browsing, as well as via an API and a SPARQL endpoint for more technical access. In this talk, we introduce a new chatbot interface that allows users to interact with the Knowledge Graph using natural language. This provides an additional, user-friendly entry point and broadens access to mathematical research data.

Presenter: Dr CONRAD, Tim (ZIB, MaRDI)

Session Classification: Tool Demos

Contribution ID: **6**   Type: **not specified**

NOMAD: a federated ecosystem for AI-ready data

Presenter: Dr MÁRQUEZ PRIETO, José A. (Humboldt Universität, FAIRmat)

Session Classification: Tool Demos

Contribution ID: **7**   Type: **not specified**

Automated Workflows and Machine Learning for Materials Science Simulations

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 tool-demo, we provide an 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 demo gives a general introduction to the use of Pyiron with a focus on atomistic simulation tasks. As a practical example, the relevant steps of the workflow for the construction of ab initio phase diagrams will be demonstrated, with the focus on the training and validation of machine learning potentials that are used for this purpose.

Presenter: Dr HICKEL, Tilmann (BAM, MatWerk)

Session Classification: Tool Demos

Contribution ID: **8** Type: **not specified**

Wikidata: Wikimedia's knowledge graph in a world of generative AI

Presenter: ANG, Alan (Wikidata)

Session Classification: Keynote talk 1

Contribution ID: **9** Type: **not specified**

NFDI4DS: Search and Explore Research Artifacts

The talk gives an overview of the NFDI4DS Portal to search and explore research artifacts

Presenter: Prof. SCHIMMLER, Sonja

Session Classification: Tool Demos