Leibniz ScienceCampus
Digital Transformation of Research

The Impact of Digitalisation on Science: Workflows, Outputs, and Trust

Tandem Talk

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Agenda

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1. Introduction to DiTraRe (Leibniz Science Campus)
2. Short history of digitalisation in science
3. AI in science: public trust & research integrity
4. Use case example: Smart Labs & AI
5. Conclusions & open questions

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In **DiTraRe** we investigate the effects and potential of the digitalisation of scientific work with a focus on:

- collection of research data,
- organisation of knowledge & use of AI,
- handling of sensitive data,
- publication cultures.

Based on specific questions (use cases), research clusters develop solutions and dimensions work on cross-cutting topics.

In this talk we focus on 2 of our dimensions (*reflection & resonance*, *tools & processes*) and 1 research cluster "*smart data acquisition*" with the use case "*chemotion electronic lab notebook*"

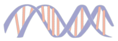
Short history of digitalisation in science

1703 — **Leibniz develops the Logical Machine, binary number system.** Publishes *Explication de l'Arithmétique Binaire*

1936 — **Alan Turing** publishes "*On Computable Numbers*", introducing the **Turing machine**

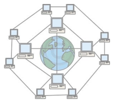
1938 - 1977 — **Introduction of computers and application in Research**

- 1938-1941 — First computers by Konrad Zuse: Z1 (1938, binary mechanical), Z3 (1941, first digital computer).
- 1945 — Von Neumann Architecture
- 1975 — First Personal Computers: Altair 8800 (1975) Intel's 8080 processor, Apple I (1976), Commodore PET (1977), …
- 1977 — First computational DNA sequencing



1970s-1980s — **Networking & the Internet and early internet protocols.**

- 1969 — ARPANET goes online, connecting four U.S. universities (UCLA, Stanford, UCSB, University of Utah).
- 1983 — Internet (TCP/IP protocol) is standardised.
- 1989 — WWW: Tim Berners-Lee launches the World Wide Web, revolutionising information access (web browsers…)



1990s — **Open Science movement -** enhances transparency and accessibility. e.g.: 1991 arXiv.org starts

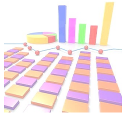
- 2001 — Open Knowledge, platforms like Wikipedia democratise knowledge and enable collaborative content creation.

2000s — **Digitisation of Libraries starts**

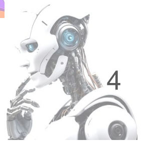
- 2002 — Internet Archive's Million Book Project starts (still relevant: Websites and data disappear - e.g. now in the US)
- 2004 — Google and major libraries begin digitising books at scale (Project Gutenberg already started in 1971)

2000-2010s — **Data-Driven Research advances**

- 2000 — Cloud computing and Big Data infrastructures transform data storage and analysis.
- 2008 — CERN's Large Hadron Collider produces vast datasets.
- 2009 — Jim Gray's Fourth Paradigm describes the era of data-intensive scientific discovery.
- 2014 — Research Tools like Electronic Lab Notebooks (ELNs) improve structured data acquisition and reproducibility.



recent years — **Artificial Intelligence (AI) & Machine Learning (ML) become central to scientific data analysis**



Short history of digitalisation in science

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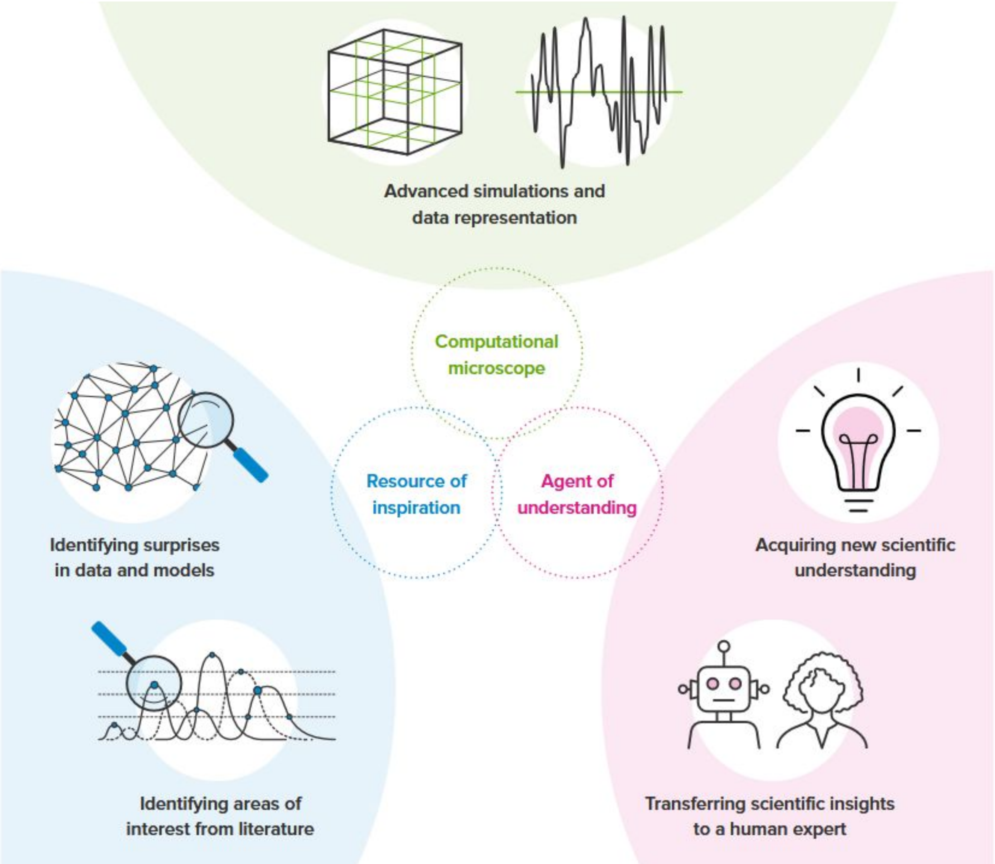
Today: Potential contribution of AI to scientific understanding



From: The Royal Society (2024): Science in the age of AI: How artificial intelligence is changing the nature and method of scientific research., p. 31

Public trust & research integrity

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- **Digitalisation of research affects how science is conducted but also how it is perceived**
  - Transparency, data openness, and the potential for reproducibility enhance public trust.
  - The reliance on black-box AI systems and large-scale datasets raises concerns about the reliability and accessibility of scientific findings
- **(Generative) AI challenges workflows, infrastructures and outputs in science**
  - New chances for knowledge generation and processing
    - Increased efficiency and productivity in scientific working practices with various possible applications
    - Potentials in training small data sets, LLM-based knowledge extraction from data bases, easier programming tools
  - But:
    - Technical limits: Transparency and traceability: detection, authentication, "hallucinations"
    - Social changes: AI-literacy of researchers & potential loss of competences
    - Legal issues: Data protection, limits of regulation
    - Ethical questions: Overreliance, spread of false information, biased knowledge, source misrepresentation
- **Challenges on two levels → focused on in this talk**
  - Trust in science from the public
  - Research integrity within science

Public trust & research integrity

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Trust in science from the public

- Narratives of low public trust in scientists, but no empirical evidence, e.g. by recent international 68-country survey
  - In most countries, scientists and scientific methods are trusted.
  - Factors e.g. being male, conservative, science-populist attitudes, are correlated with lower trust

- Four components of trust in scientists: competence, **integrity**, benevolence and **openness**
  - Public perception of integrity is high → **risk of erosion by AI in science?**
  - Public perception of openness is lower → **how to deal with it in case of AI & open data?**
    - receptive to feedback, transparent about funding and data sources
    - communicating about science with the public, avoiding top-down communication
    - encouraging public participation in genuine dialogue, insights and needs of societal actors

Cologna, V., Medreertertere, N.G., Berger, S. *et al.* Trust in scientists and their role in society across 68 countries. *Nat Hum Behav* (2025). https://doi.org/10.1038/s41562-024-02090-5

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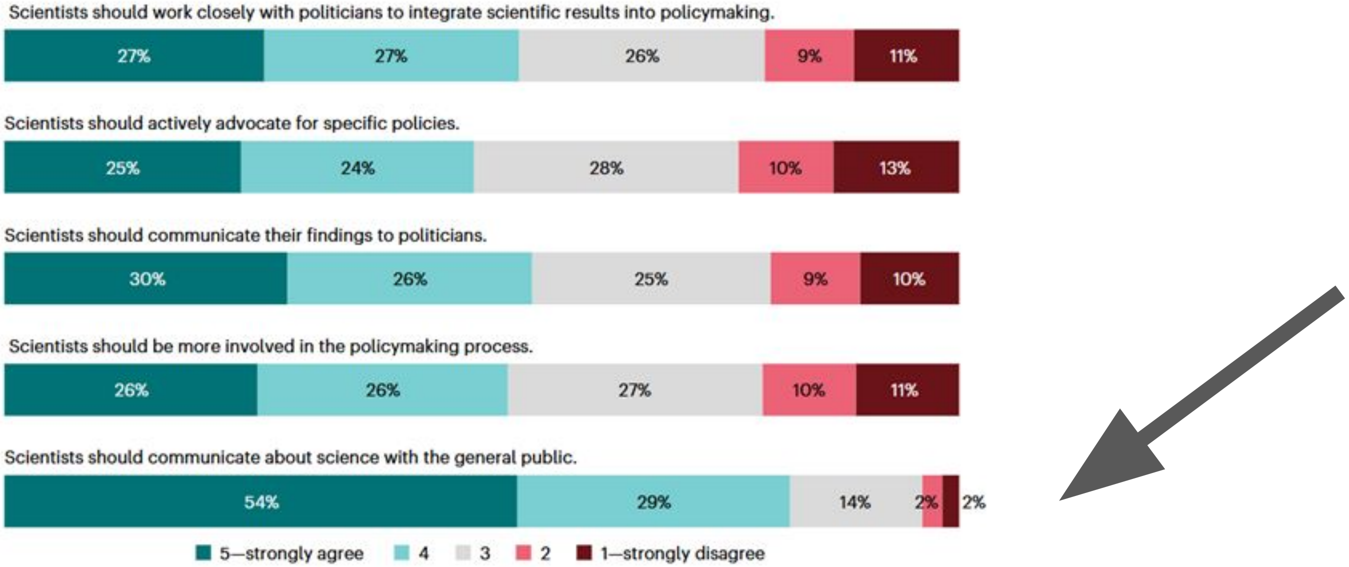

Fig. 4 | Normative perceptions of scientists in society and policymaking. Normative perceptions of scientists in society and policymaking using weighted response probabilities.

Cologna, V., Medreertertere, N.G., Berger, S. *et al.* Trust in scientists and their role in society across 68 countries. *Nat Hum Behav* (2025). https://doi.org/10.1038/s41562-024-02090-5

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Trust in science from the public - Open Science

Table 1. Survey questions (Study 1).

ID	Wording	Response format	*M*	*SD*	Positive responses (%)
SQ1	How important do you think it is that scientific results are made available to the public free of charge (e.g., on the Internet)?	7-point scale, *not important at all* to *very important*	5.96	1.19	87.2
SQ2	How important do you think it is that the following scientific results are made available to the public free of charge (e.g., on the Internet)? • SQ2c: Study materials, datasets, and analysis code of individual studies	7-point scale, *not important at all* to *very important*	5.09	1.32	64.3
SQ3	My trust in a scientific study increases when I see scientists publicly sharing their study materials, their datasets, and their analysis code.	7-point scale, *do not agree at all* to *fully agree*	5.25	1.26	74.0

Rosman, T., Bosnjak, M., Silber, H., Koßmann, J., & Heycke, T. (2022). Open science and public trust in science: Results from two studies. Public Understanding of Science, 31(8), 1046-1062. https://doi.org/10.1177/09636625221100686

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Trust in Science from the public - Open Science and AI

- Measures for trust in open data using AI
  - Improve reproducibility of AI-based research
    - requesting the use of reproducibility checklists and data sharing protocols
    - supporting the development of community and field-specific reproducibility standards
  - Invest in open repositories
    - sharing of datasets, software versions, and workflows
    - development of context-aware documentation that enable the local adaptation of AI models across research environments
  - Trustworthy use of sensitive datasets
    - relates to people (e.g. health information, demographics, location, etc.).
    - trusted and secure research environments that enable sensitive data sharing (--> *other use case*)

The Royal Society (2024): Science in the age of AI: How artificial intelligence is changing the nature and method of scientific research., p. 13;

Public trust & research integrity

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Research integrity within science: National guidelines (DFG)

- **“The use of generative models** in the context of scientific work **should by no means be ruled out** in view of the considerable opportunities and development potential. However, their use requires certain binding framework conditions in order to ensure good scientific practice and the quality of scientific results.”

- **“Transparency and traceability** of the research process and the knowledge gained for third parties are essential basic principles of scientific integrity. This value system continues to provide valuable guidelines for dealing with generative models.”

- “Scientists should **disclose whether and which generative models they have used**, for what purpose and to what extent, **when making their results publicly available in the interests of scientific integrity.”**

- “The influence of generative models on the sciences and the DFG's funding activities can currently only be partially recognised. In order to illuminate the opportunities and challenges, **it is necessary to gather and share experiences with the use of generative models. Only this will enable a discursive and science-based process.”**

DFG (2023): Stellungnahme des Präsidiums der Deutschen Forschungsgemeinschaft (DFG) zum Einfluss generativer Modelle für die Text- und Bilderstellung auf die Wissenschaften und das Förderhandeln der DFG https://www.dfg.de/resource/blob/289674/ff57cf46c5ca109cb18533b21fba49bd/230921-stellungnahme-praesidium-ki-ai-data.pdf

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Research integrity within science*:* International guidelines

“...the usage processes should ensure humans’ interactive engagement with GenAI and higher-order thinking, as well as human accountability for decisions related to the accuracy of AI-generated content, and their impact on human behaviours” p. 29

Springer

“Large Language Models (LLMs), such as ChatGPT, do not currently satisfy our authorship criteria”

ELSEVIER

“Where authors use generative AI and AI-assisted technologies in the writing process, these technologies should only be used to improve readability and language of the work.“

“…publishers and researchers at all stages of their careers are essential in shaping the discussion on AI and how it can serve the public interest in research.” (EC 2024, S.4)

UNESCO (2023): https://www.unesco.org/en/articles/guidance-generative-ai-education-and-research
EC (2024): https://research-and-innovation.ec.europa.eu/document/2b6cf7e5-36ac-41cb-aab5-0d32050143dc_en
Elsevier (2025): https://www.elsevier.com/about/policies-and-standards/the-use-of-generative-ai-and-ai-assisted-technologies-in-writing-for-elsevier
Springer (2025):https://www.springer.com/gp/editorial-policies/artificial-intelligence--ai-/25428500?srsltid=AfmBOopzRsbwsT9pkaJbJPXq-lWMhiA8NQi_Gp9swQ5mEadFkJefjQP1

Use Case: Smart Data Acquisition -
Electronic (?) Lab Notebooks (ELN)

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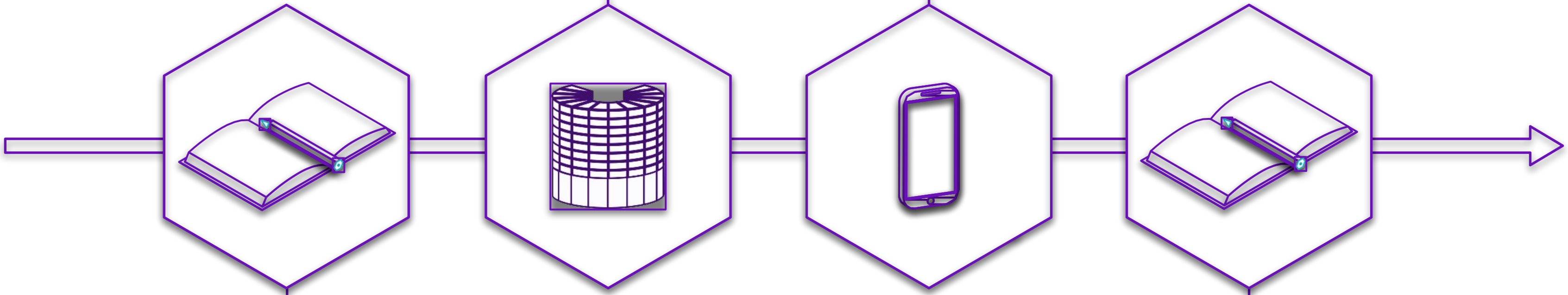
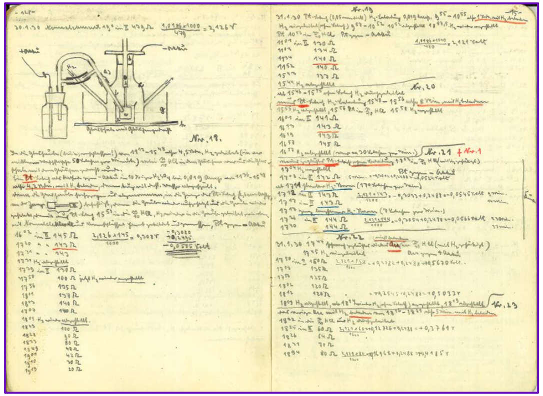
1985 2025

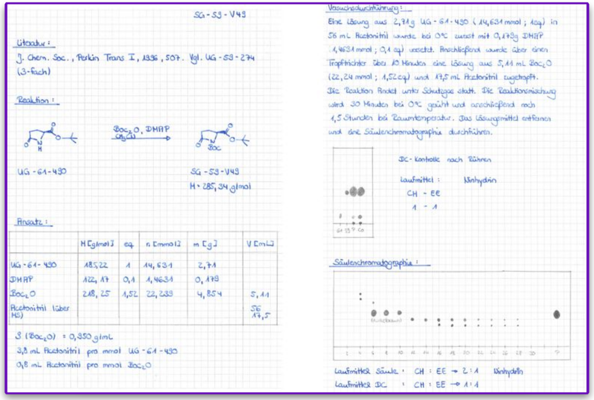


1927 2025



Cray-2, 1985
1,9 GFlops
244 MHz CPU Speed

iPhone 15 Pro
2.147 GFLOPS
3.78 GHz CPU Speed



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ENHANCE YOUR DATA.

Use Case: Chemotion - Workflow

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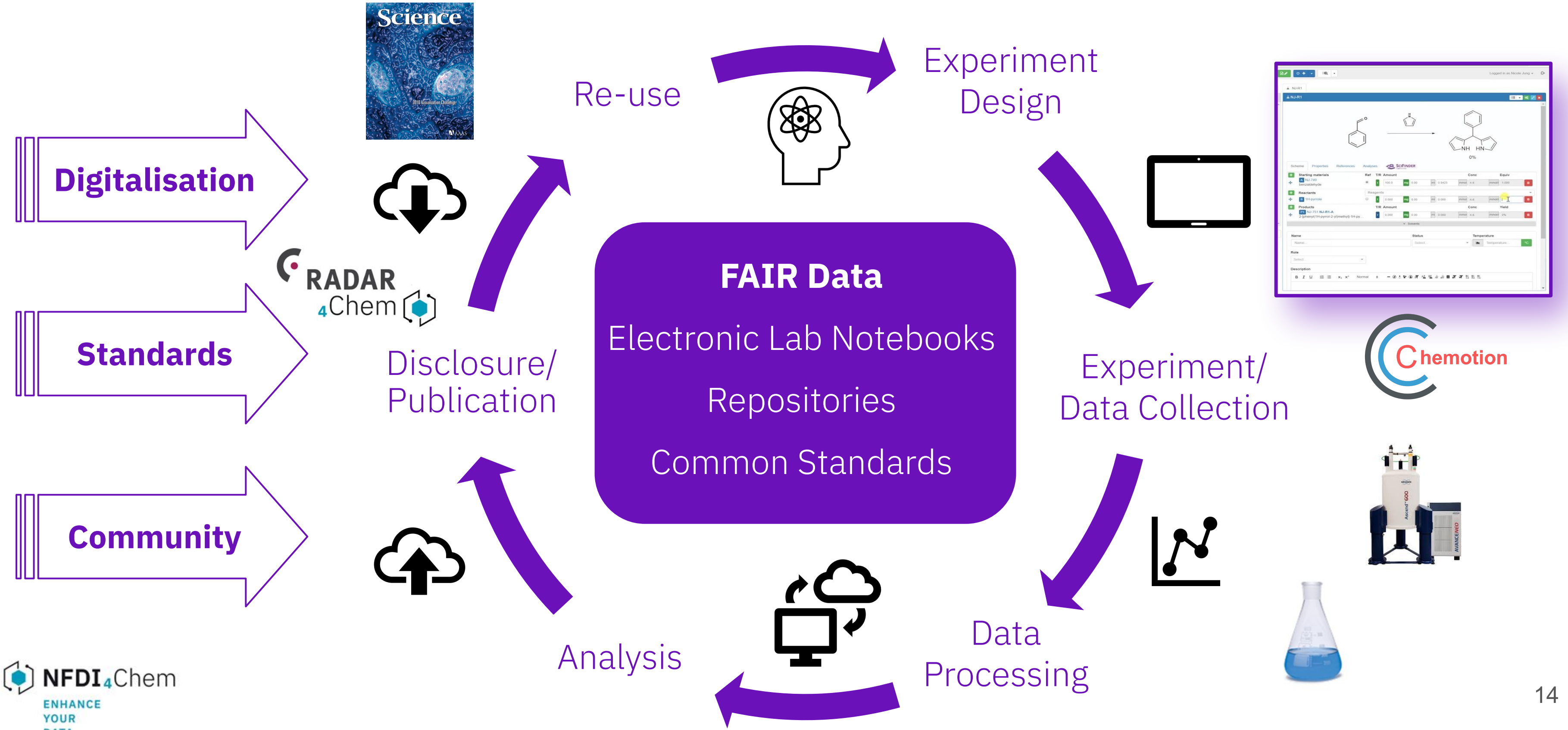

Use Case: Electronic Lab Notebook

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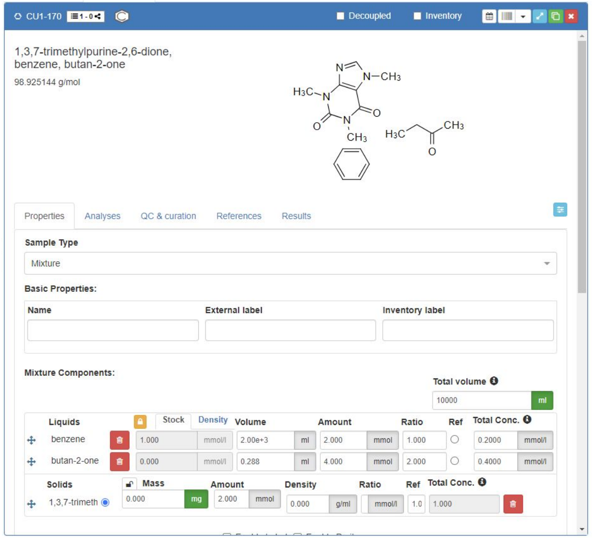
Chemotion ELN: A Major Digitalisation Achievement (NFDI4Chem, KIT-IBCS)



Chemotion

- Standardisation & Interoperability
- Improved Reproducibility
- Automated Data Logging & Organisation
- Enhanced Collaboration
- FAIR Principles Compliance
- Regulatory & Compliance Benefits

4. AI use in Chemotion ELN

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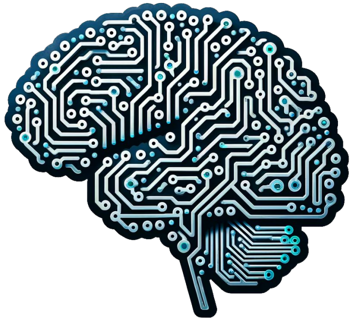
Potential AI Benefits for Data & Metadata Curation in Chemotion

- Automated Metadata Extraction
- Smart Data Classification & Tagging
- Predictive Data Cleaning & Error Detection
- AI-Assisted Data Retrieval & Querying
- Machine-Generated Reports & Insights



Reflections – AI in Open Research Data

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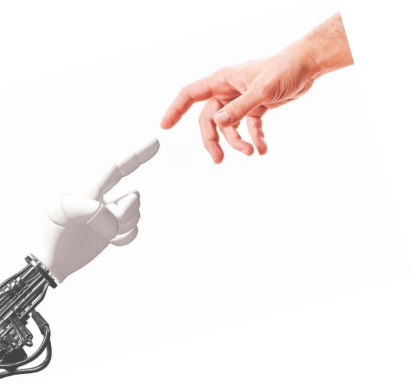

- Strengthening Open Data
  - AI improves metadata quality, small dataset utilisation, and collaboration.
  - Acts as a virtual research assistant.
- Human-AI Collaboration
  - Defining the role of human verification in research.
  - Limits of "human-in-the-loop" approaches?
- Changing Knowledge Processes
  - Shift from control knowledge → translational knowledge.
- Standards & Governance
  - Guidelines vs. AI progress – addressing the Collingridge dilemma.
  - Bottom-up vs. top-down: Who should drive AI standards?
- Implementation Challenges
  - Ensuring scalable, effective AI integration in research.

Digital Science (2023): The State of Open Data 2023. Digital Science. Report. https://doi.org/10.6084/m9.figshare.24428194.v1

Conclusions

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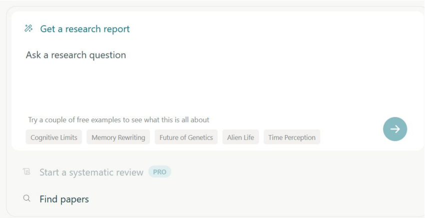
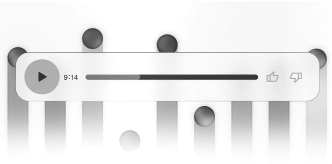
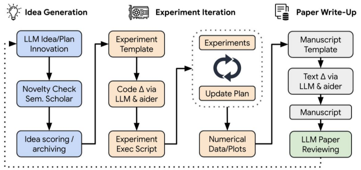


- ## Opportunities
  - **AI-based research assistant** (e.g. Elicit)
  - **Conversational access to science** by AI summarised texts & podcasts (e.g. Google Notebook LM)
  - Full replacement of scientific discovery: “The **AI scientist**” (e.g. Sakana AI)
- ## Challenges
  - **Research integrity** within science → continuous development
    - **Explainable AI/human in the loop**: transparency but limits of human verification → **Bias** remains
    - Role of **guidelines** - limits of guidelines



  - **Trust in science** from the public → increase of openness
    - **Communication** formats with the public on genAI use in science & open research data
    - Inclusion of **stakeholders** in the assessment process (e.g. publishers, funding, data & rights protection)
- ## Risks
  - **Disappearance of Data** hosts & access to tools may be limited → *https://safeguarding-research.discourse.group/*
  - Limits of co-hosting data in Europe → not all data can be covered
  - Source of genAI data → trustworthiness of national tools (e.g. Open AI vs. Deep seek)



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Further questions?

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