MatCHMaker
Materials Characterisation & Modelling

Workshop on Data Life Cycles in the World of Materials Modelling and Characterisation

TU Wien, 7th April 2025, 13:00 – 18:00

Introduction to the Workshop

Nadja Adamovic, TU Wien/EMMC ASBL

Workshop Background

- Horizon-CL4-2022-RESILIENCE-01-19: Advanced materials modelling and characterisation (RIA)
- Projects Involved: MatCHMaker, AddMorePower, Aid4Greenest, CoBrain, D-STANDART, KNOWSKITE-X
- Common Thread: Managing vast amounts of data across its lifecycle—from creation to knowledge extraction

Workshop Objectives

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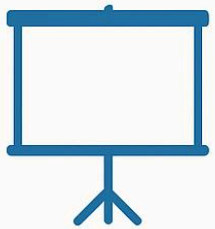

Project Presentations:

Brief talks by project representatives on how they address each stage of the data life cycle

Key Discussion Points:

Planning
How data needs are determined and managed

Acquisition
Methods for data capture and metadata collection

Processing
Extraction and workflow automation

Analysing
Tools and approaches for extracting knowledge

Preserving & Sharing
Data documentation, versioning, repository choices, and sharing protocols

Survey Findings & Identified Challenges

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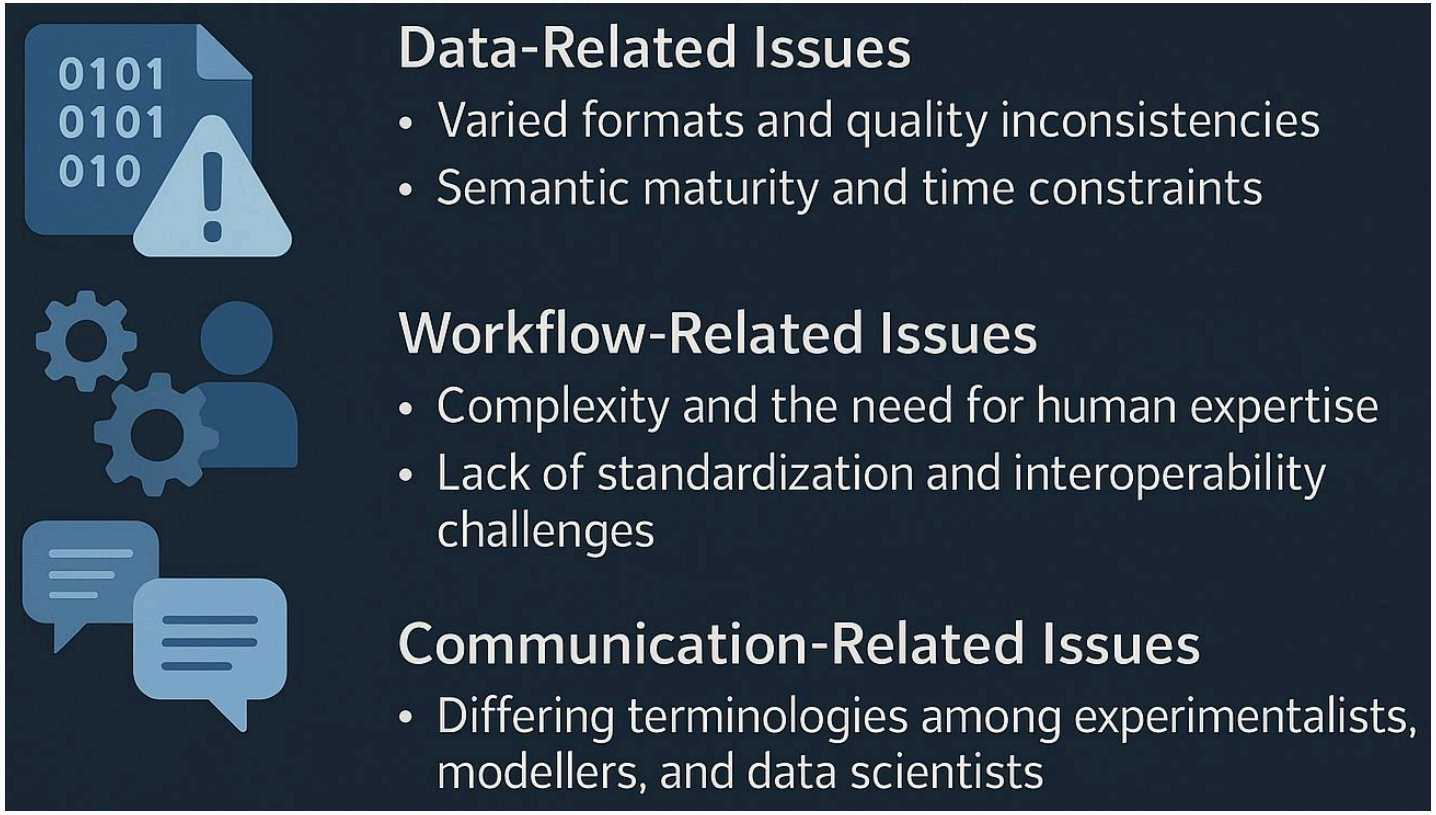

Bottlenecks in the Data Life Cycle

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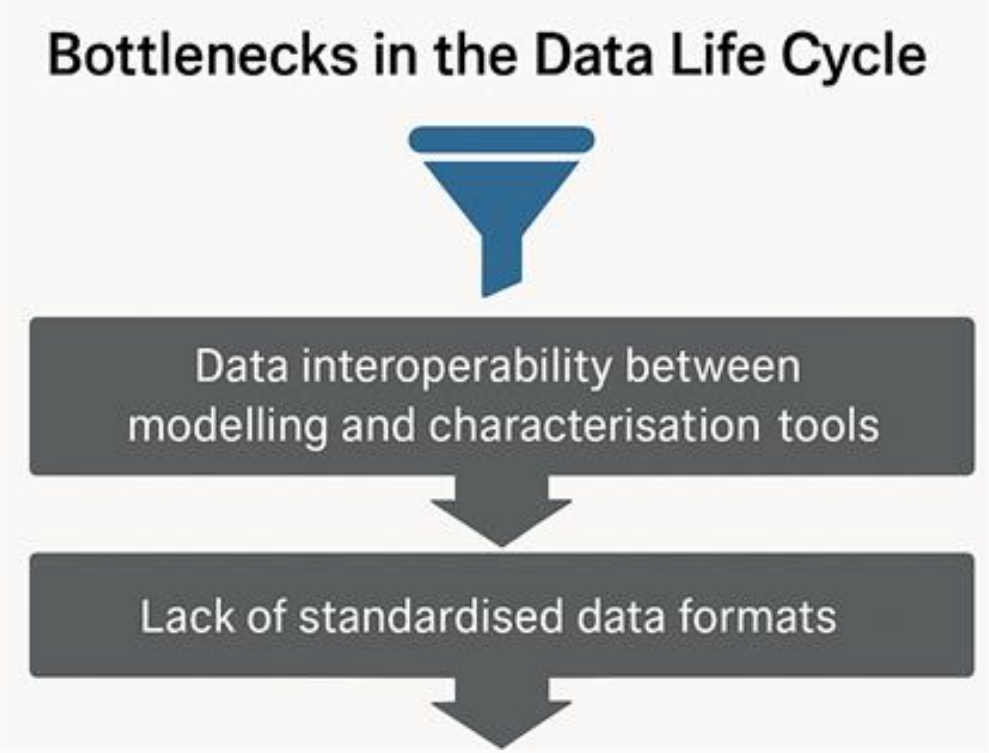

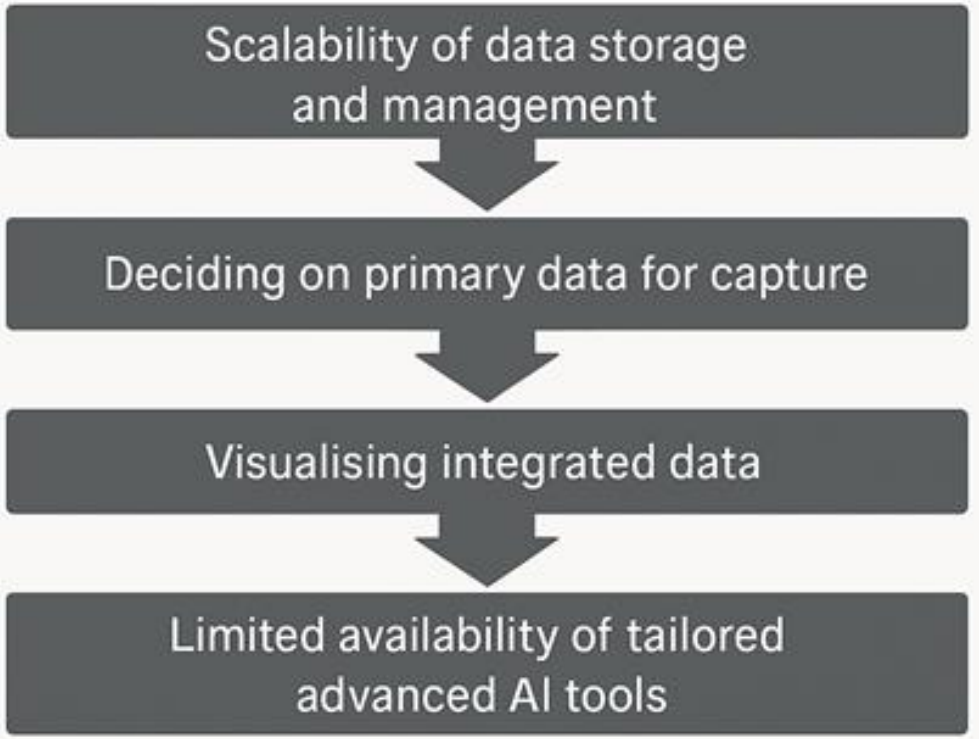

Interactive Homework – Your Input Needed!

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- Questions for You:
  - Do you encounter these **challenges** in your own data life cycle?
  - Can you suggest **additional hurdles** or even **potential solutions**?
  - What **benefits** do you see in **integrating robust data life cycle practices in R&D**?

Workshop Schedule Overview

- Agenda Highlights:
  - Registration and Networking
  - Opening & Welcome
  - **Project Talks** covering key aspects from data life cycle
  - Coffee break and group photo
  - Final session for **discussion and networking**

Conclusion & Looking Forward

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- Key Takeaways:
  - Integration of modelling and characterisation data remains challenging yet essential
  - Collaborative discussion can spark innovative solutions
  - Your feedback is vital – both during and after the workshop
- Invitation:
  - Let’s use today’s session to pave the way for more interoperable, effective data workflows in materials science.

Q&A / Transition to Presentations

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Time	Actor	Topic
12.00 – 13.00	all	Registration and Networking
13.00 – 13.15	Nadja Adamovic (TU Wien, AT) - MatCHMaker	Welcome & Introduction
13.15 – 13.45	Alexandre Ouzia (Heidelberg Materials, DE), Geoffrey Daniel (CEA, FR) and Sophie Schmid (TU Wien, AT) - MatCHMaker	Characterization and modelling data workflows for low carbon cement optimisation
13.45 – 14.15	Yoav Nahshon (Fraunhofer IWM, DE) - AID4GREENEST	Interoperable CHADA: A Semantic Approach for Managing and Exploiting Characterization Data and Protocols
14.15 – 14.45	Julian de Marchi (NLR-Netherland Aerospace Centre, NL) – D-STANDART	Case study: CHADA v2 population with materials characterization data from the D-STANDART project

Thank you!

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