The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators

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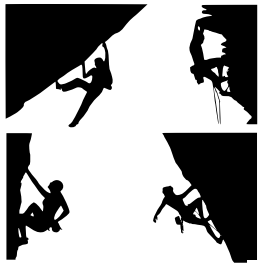
Integration of ELNs in scientific research

School of Geography, Earth and Environmental Sciences,
University of Birmingham, UK

ELN Hackathon
July 2020

Data Driven Innovation

Disturbance



Data Collection

Data Analysis

Impact

Innovation, Growth
Entrepreneurship

New Insights

Novel solutions
and services

Planning

There is only a finite amount of iterations that can be performed with restricted data!

Data Driven Innovation – Barriers

1. Lack of a systematic process
2. Problems with data access
3. Lack of appropriate digital tools
4. Insufficient competence
5. Data is rarely used as a strategic resource
6. Lack of (e-)infrastructure investment

Challenges Concerning Data Driven Innovation, Cronholm et al., Australasian Conference on Information Systems, 2017, Hobar

Data Management

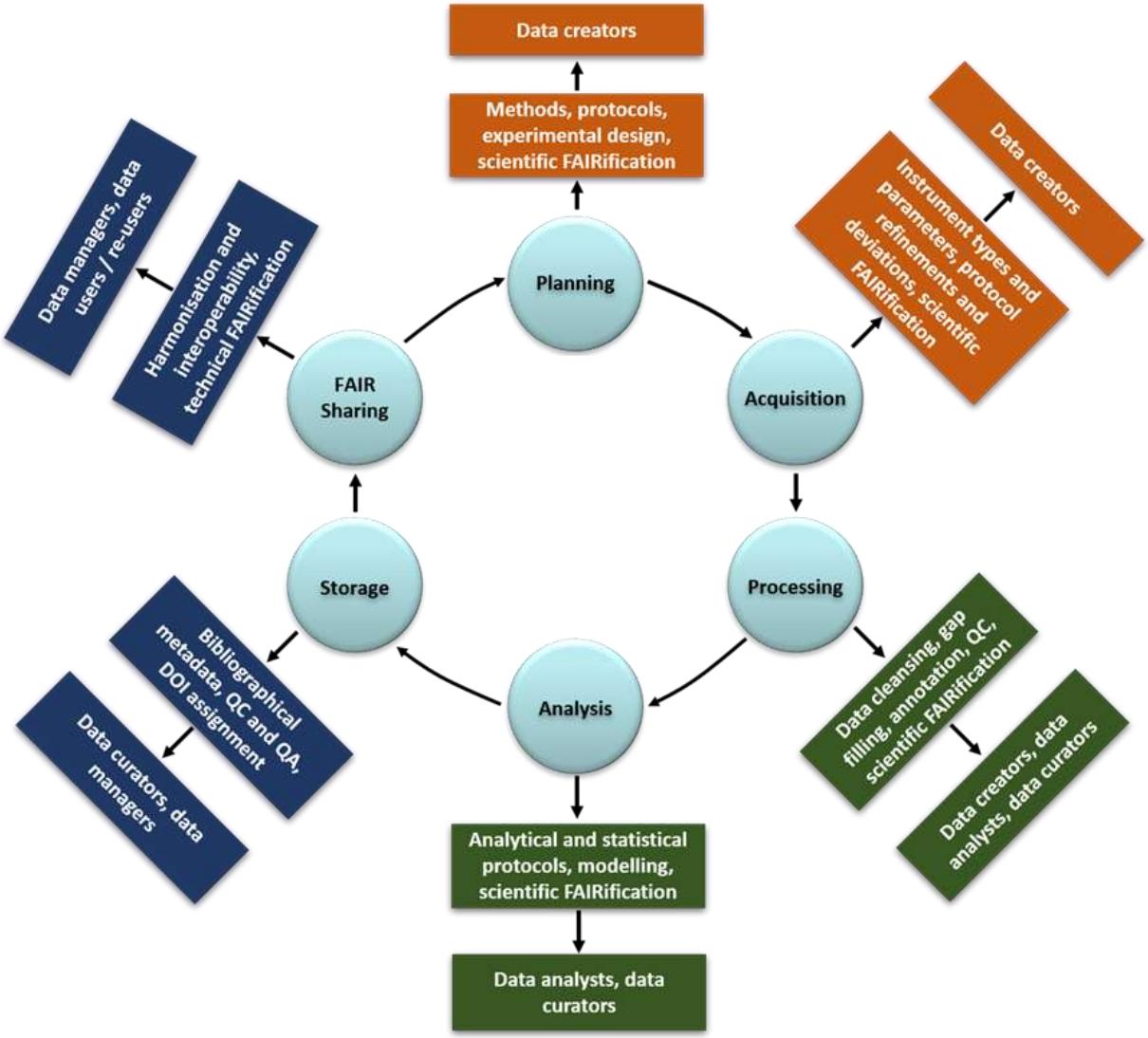
Definition

Data Management is the implementation and application of processes, which allow the acquisition, storage, manipulation and analysis of data during its lifecycle.

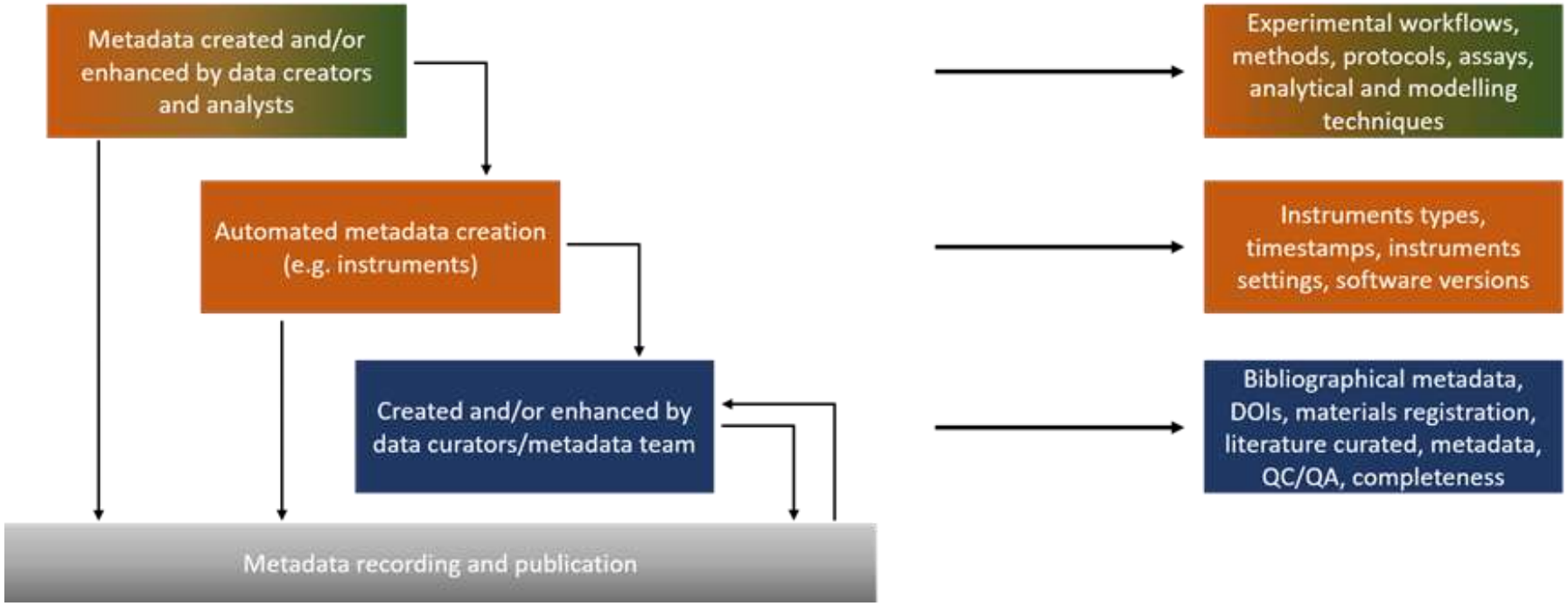
Cause & Effect

- Is the most neglected scientific process
- Most labs, at a global scale, are yet to enter the 21st century
- Can lead to significant loss of data and metadata
- Can decrease the quality of data and scientific publications
- Can lead to the loss of significant insights
- Does not allow further data exploitation (e.g. AI, machine learning)

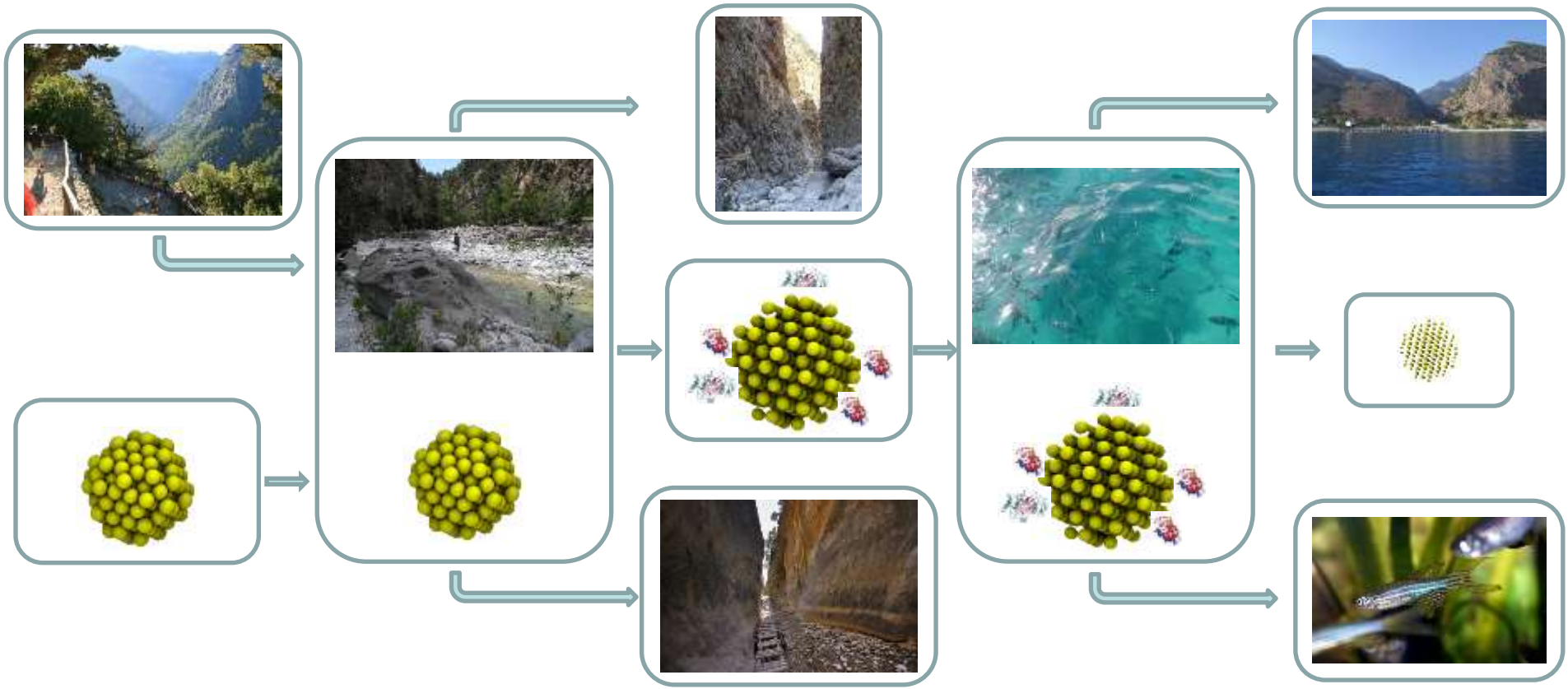
Data management, data lifecycle & metadata



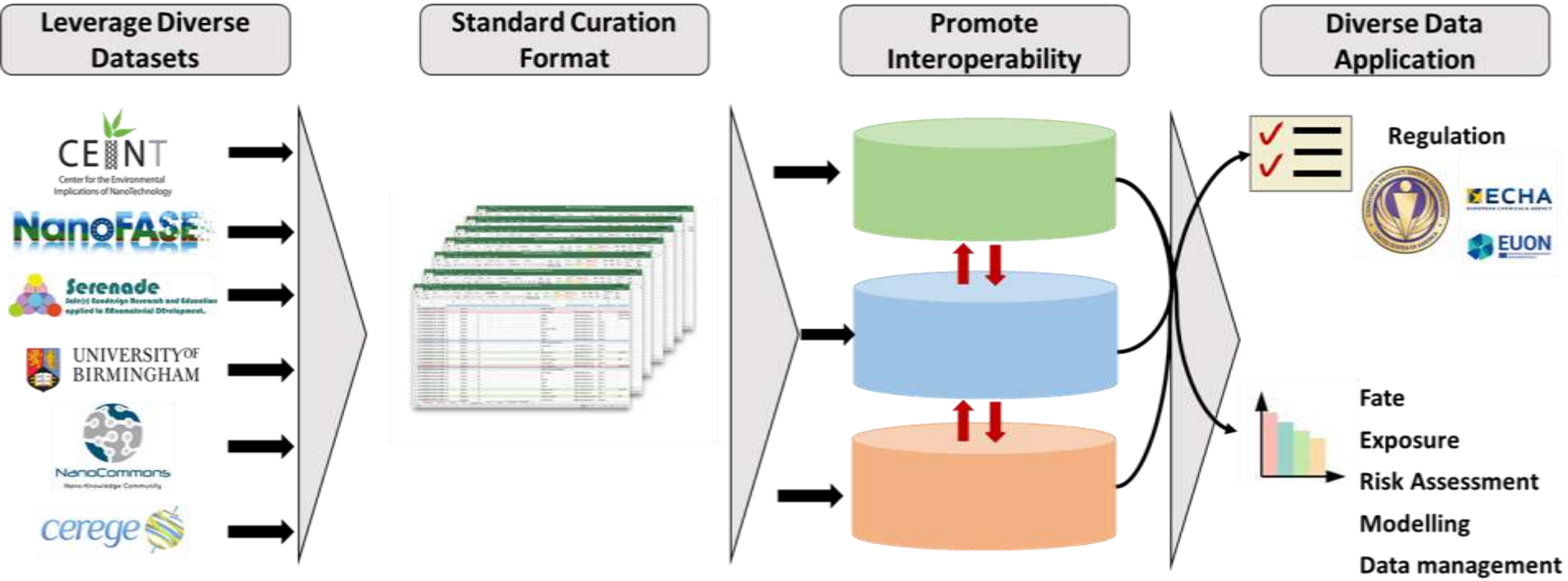
Metadata Implementation



Exposure & Fate Case Study

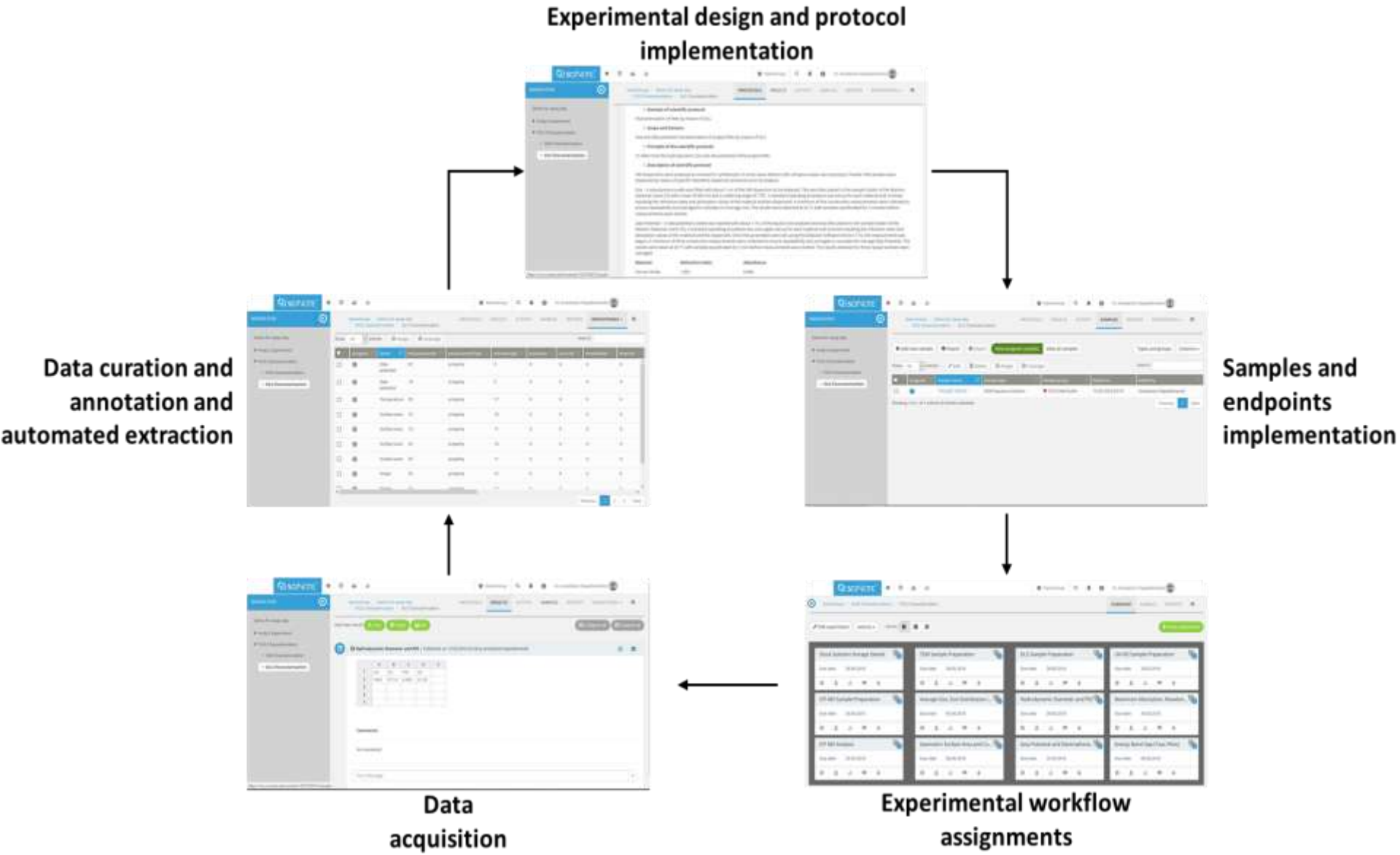


Data Curation & Interoperability



- **Bridge different fields by promoting data comparability and project continuity**

ELN Data Acquisition & Management



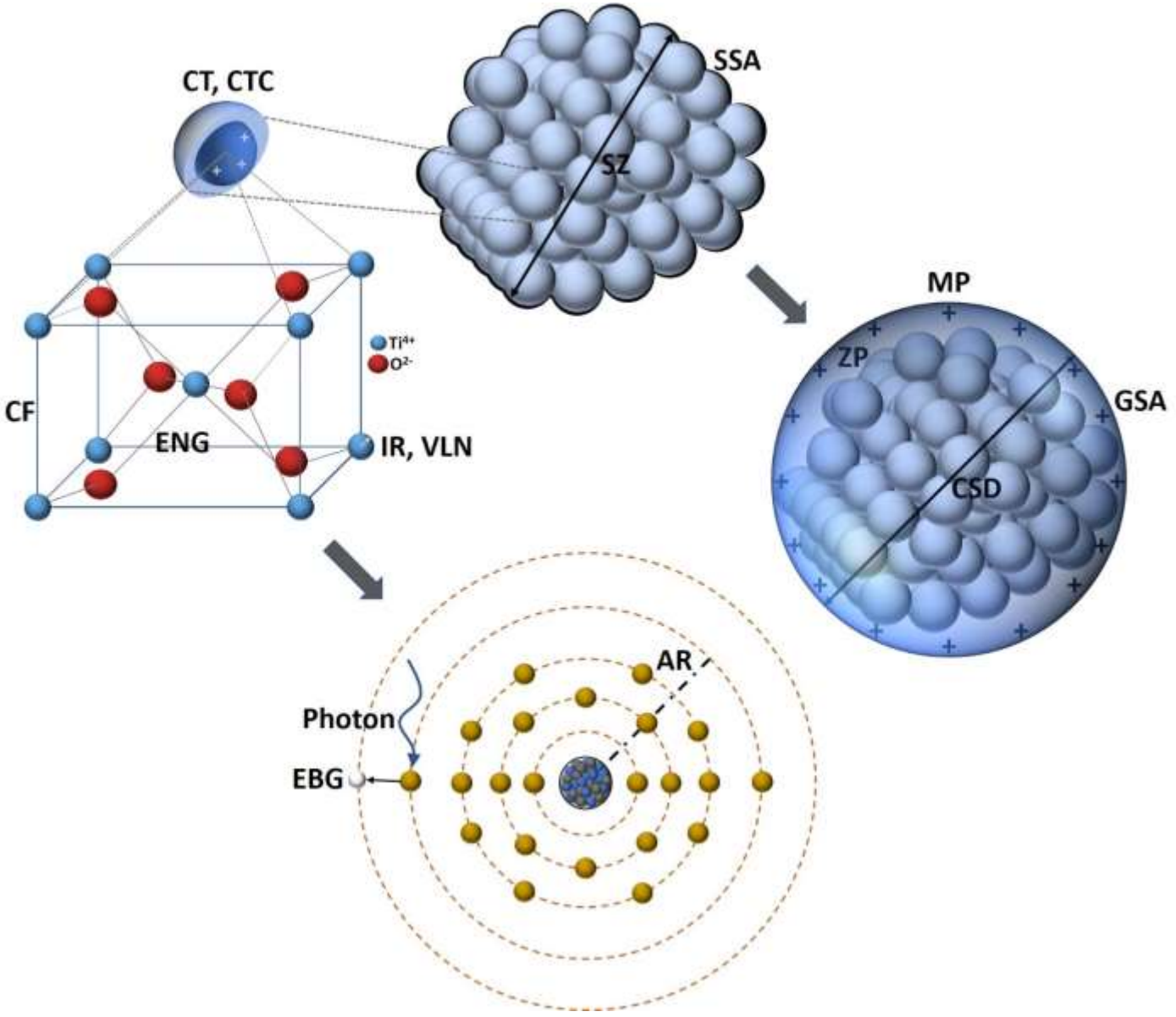
Why ELNs

- **Providing a complete data management environment**
- **Complex workflow support, web services, digital and electronic sign off, analysis and reporting capabilities**
- **Flexible enough to support automation of personalised adaptive workflows**
- **Workflow standardisation and template configuration for every experiment performed within a group/organisation**
- **Capturing of all appropriate metadata and QC of results**
- **An eco-friendly ways to reduce the amount of paper a laboratory consumes**

ELNs vs. LIMS

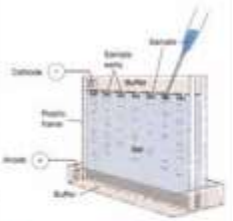
- **LIMS is a rigid sample-centric information management system**
- **User must follow a pre-defined rigid workflow enforced through the LIMS, allowing an organisation to track samples and compile reports of data generated against samples or batches**
- **LIMS lack the ability to capture ‘context’**
- **LIMS workflow tends to be structured by management and IT making it less adaptive**
- **LIMS are better for managing structured information and ELNs are better for more disparate, unstructured information**
- **LIMS ideally suited for regulated environments**

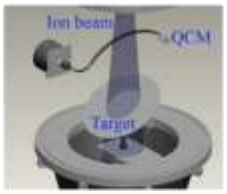
Nanomaterials Characterisation



From a Local Network…

DCS



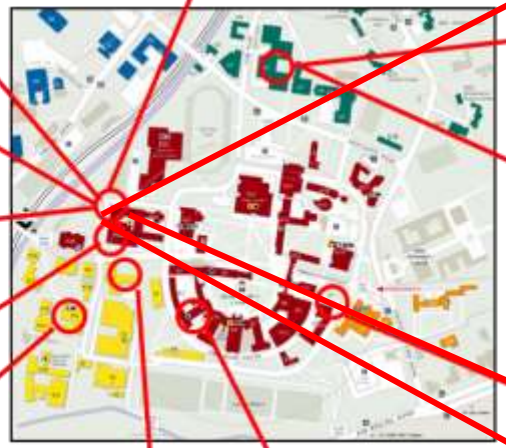


QCM

BET

Eco-interactions
(Electrophoresis, gel imaging etc.)

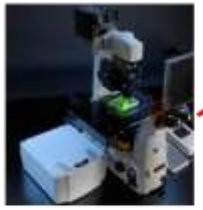
FFF



TEM
(+ EDS, EELS)

DLS
Zeta potential

SEM,
ESEM



Confocal

AFM

NTA

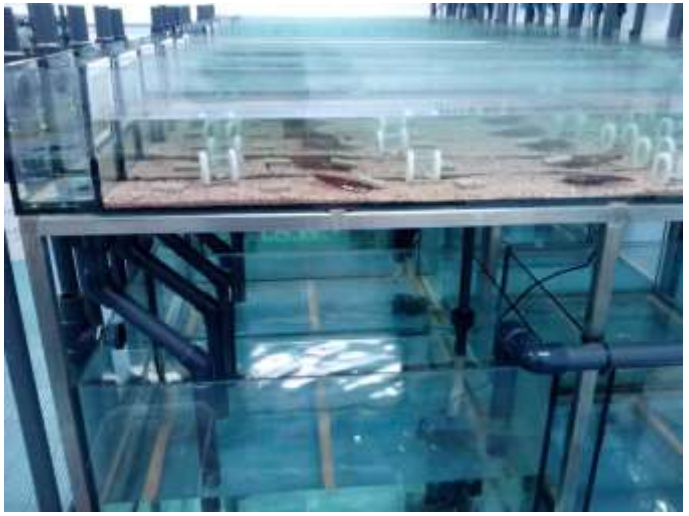
XRD

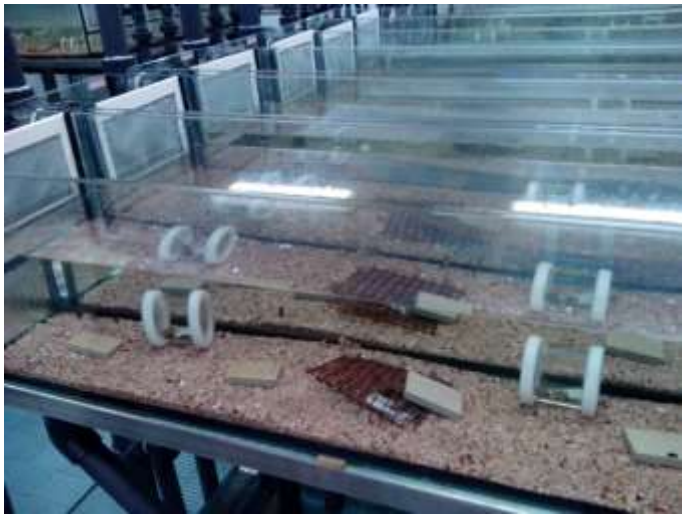
ICP-MS
Sp-ICP-MS
ICP-AES
Sc-ICP-MS

UV-VIS

ELN Data Acquisition & Management

Aquatic Mesocosm Experiments





36 units (rivers)

Terrestrial Mesocosm Experiments

30 mesocosms

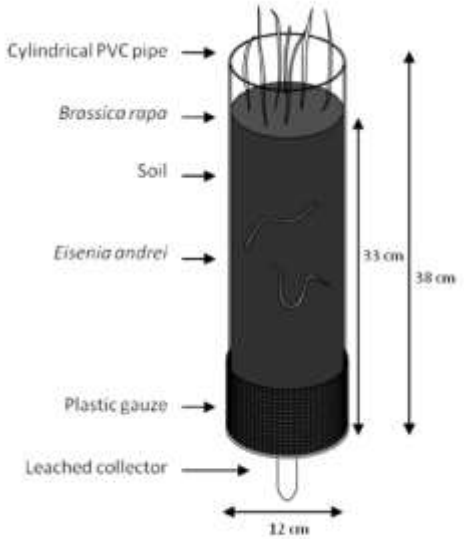


Fig. 1. Small-scale terrestrial ecosystem (STEM) used in the experimental procedure.

… to a Wide Network

- **Aquatic and terrestrial mesocosm experiment, 7 EU countries and 10 Institutions**

To a Wide Network…

NanoCommons
Nano-Knowledge Community

ID	measurementId	measurementType	referencingId	timeRelative	timeUnit	timeAbsolute	parameter	inheritId	parameterDescription	parameterDataType	parameterText	parameter
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	324	property	25	7	day		Kda Ag		Kda Ag 52	numeric		
	325	property	25	7	day		Kda Ag		Kda Ag 53	numeric		
	326	property	25	7	day		Kda Ag		Kda Ag 54	numeric		
	327	property	25	7	day		Kda Ag		Kda Ag 55	numeric		
	328	property	25	7	day		Kda Ag		Kda Ag 56	numeric		
	329	property	25	7	day		Kda Ag		Kda Ag 57	numeric		
	330	property	25	7	day		Kda Ag		Kda Ag 58	numeric		
	331	property	25	7	day		Kda Ag		Kda Ag 59	numeric		
	332	property	25	7	day		Kda Ag		Kda Ag 60	numeric		
	333	property	25	7	day		Kda Ag		average Kda Ag	numeric		
	334	system	21				name			text	NM	
	335	property	334	7	day		diameter		diameter	numeric		
	336	property	334	7	day		diameter		diameter	numeric		
	337	property	334	7	day		diameter		average diameter	numeric		
	338	property	334	7	day		microbial community		microbial community (clean)	text		
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	346	property	334	7	day		microbial community		microbial community (clean)	text		
	347	property	334	7	day		microbial community		microbial community (clean)	text		

- **> 10,000 data points**

… and Global Network

Support for customised experimental workflows of varying complexity, … to wide area networks (WAN)

ACEnano round robins

Conclusions

- **Data is a main driver of innovation**
- **Data Management is the most neglected, but highly significant experimental process with multiple applications**
- **Data curation needs to be taken down to data generators and automated**
- **ELN can help with this due to their flexibility and personalisation potential (compared to LIMS)**
- **Facilitate dataset QC, processing and analysis**
- **Can be applied from a local (single institution) to a wide (global) network to enhance harmonisation of data capture / storage**
- **Need to be expanded and directly linked with data repositories and support computational workflows (e.g. Jupyter notebooks)**

Acknowledgements

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UNIVERSITY OF BIRMINGHAM

Edelweiss Connect

CEH

NovaMechanics

Biomax INFORMATICS

U M

CEINT
Center for the Environmental Implications of NanoTechnology

BIO NANONET

UNIVERSITÄT SALZBURG

Oregon State University

LEITAT
Technological Center

UCD DUBLIN

BfR
Risiken erkennen – Gesundheit schützen

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Thank you!

Take our survey to let us know the tools the nanosafety community needs:

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