



# Nanosafety databases: harmonisation efforts in Europe

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EU NanoSafety Cluster WG4

# Objective of NSC WG4



To develop an EU-project-wide strategy for capturing and storing data emerging from EU-funded projects, thereby reducing the duplication of costs / effort in EU-funded projects for data management.

- Not a trivial task. Need to address issues around:
  - Descriptors for all aspects of materials, characterisation, impacts (tox & ecotox), exposure, LCA, modelling, QSARs etc.
  - Capture negative and positive effects
  - Data input & Quality assurance
  - IPR & data confidentiality issues
  - Design, implementation and maintenance strategies & PM
  - Build on existing best practice, be adaptable to new developments in science & regulation

# 2013 – 2 new projects



NMP.2013.1.3-2 Nanomaterials safety assessment: **Ontology, database(s)** for modelling and risk assessment

NMP.2013.1.3-3 Development of a systematic framework for **naming** and assessing **safety** of the **next generations** of nanomaterials being developed for **industrial applications**

=> Specific budget for this task, but must serve needs of the research community, i.e. the NSC members are a primary stakeholder

# Unique Opportunity for Nanosafety Community



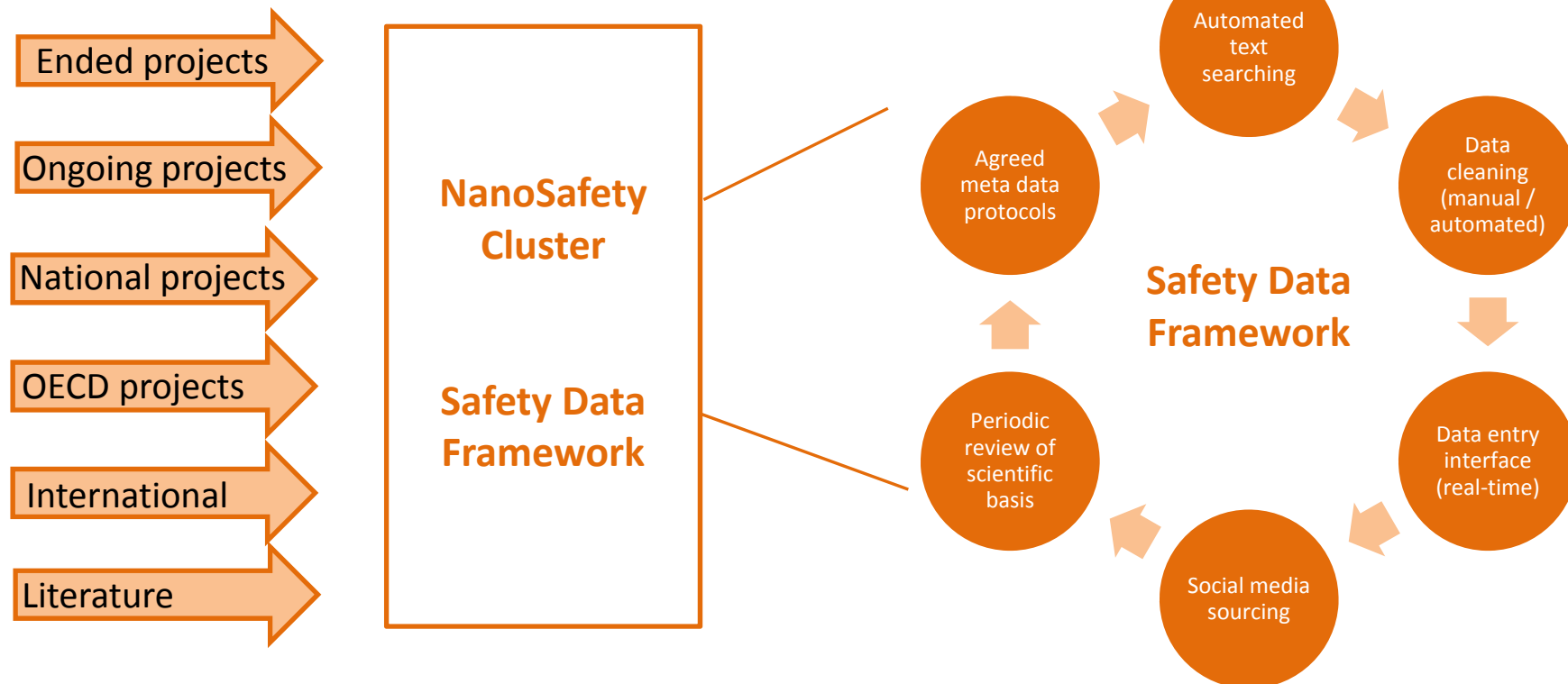
- **Gather, manage interpret current and future research**
  - Research typically 5-10 years ahead of regulation
  - Complex, unstructured data
    - properly addressed will point to broad rules for nanosafety evaluation / regulation,
    - poorly managed, lost for a decade, lost investment
- **Move Nanosafety research beyond legacy nanomaterials**
  - New complex shapes / architectures – how to describe these?
  - Radically new materials: core, shell, functionalisation & *context* matter

# Gather, manage, interpret data



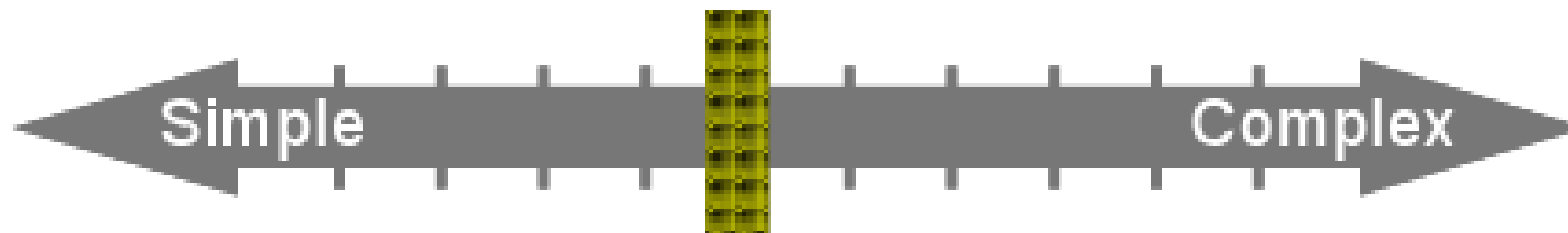
## Ontologies & Database

- Capture – link – integrate disparate & complex emerging data, where paradigm is continuously evolving
- Capture the natural dynamic and inventiveness of structures
- Capture *relevant information* (**does OECD designate quality issues or relevant parameters?**)
- Allow for identification of emerging rules/trends by search?



# How much to harmonise?

Which level of harmonisation is „just right“?



Too simple:

- identified requirements cannot be supported
- insufficient harmonisation
- few benefits

Too complex:

- difficult to implement
- substantial benefits available only to few users
- high cost

# Need agreed terminology



- Is Nanosafety = NanoEHS ?
- What does nanosafety cover?
- Can we define some agreed terms across all CoRs?

# Optimal database format

NSC WG4 meeting March 1<sup>st</sup> 2012



- For a functional and usable database there are three perspectives:
  - bench researcher,
  - modeller,
  - enterprise needs such as regulation.
- Need sufficient flexibility so that emerging / undiscovered end-points can be captured
- Need to capture exposure context & transformations



# Usability for researchers

NSC WG4 meeting March 1<sup>st</sup> 2012



- Data entry should be real-time
  - E.g. electronic notebook integration
  - This will ensure that *negative data* (i.e. where no effect is observed) is also captured
- Raw data files / qualitative information & not just the excel analysis (quantitative information)
  - for modelling & additional data extraction)
  - additional flexibility – e.g. conversion to other metrics
  - enable re-analysis of data for new purposes



# Issues around data sharing



- What will incentive researchers to share their data?
- Can we made the database citable & acknowledge contributors / funding sources?
- Can we agree guidelines for authorship / acknowledgement for work on “shared” datasets?
- Can we get publishers to support data sharing?  
E.g. proteomics and crystallography communities

# Some EU examples



- Several developed via EU FP projects
- Several national / institutional
- European Commission / JRC developed
- Several large scale data infrastructures
- Others?

# ECVAM database on alternative methods to animal experimentation



## Information content definition

- Thematic reviews by experts collecting, analysing, evaluating and synthesising wide range of agreed information sources
- Bilateral contacts between scientists and DB-ALM staff (*INVITTOX protocols*)
- Information from formal validation studies



Overall coordination and quality control of information by DB-ALM staff

## Information Content

### *In vitro* methods

	5
Topic Summaries	153
Method-Summary Descriptions	130
<i>INVITTOX</i> Protocols	63
Evaluation Studies	19
Formal Validation Studies	8431
Test Results	5100
Bibliographic References	212
Who's who in the field of alternative methods	

# The NANOhub Database

Managing information on nanomaterials



## Structure of NANOhub (and IUCLID)

- (1) The **material(s)** investigated in the project (e.g. SiO<sub>2</sub> or Ag). Data are collected and managed as agreed within a collaboration
- (2) The data are structured in chapters and subchapters (or endpoints)

## NANOhub “Chapters”

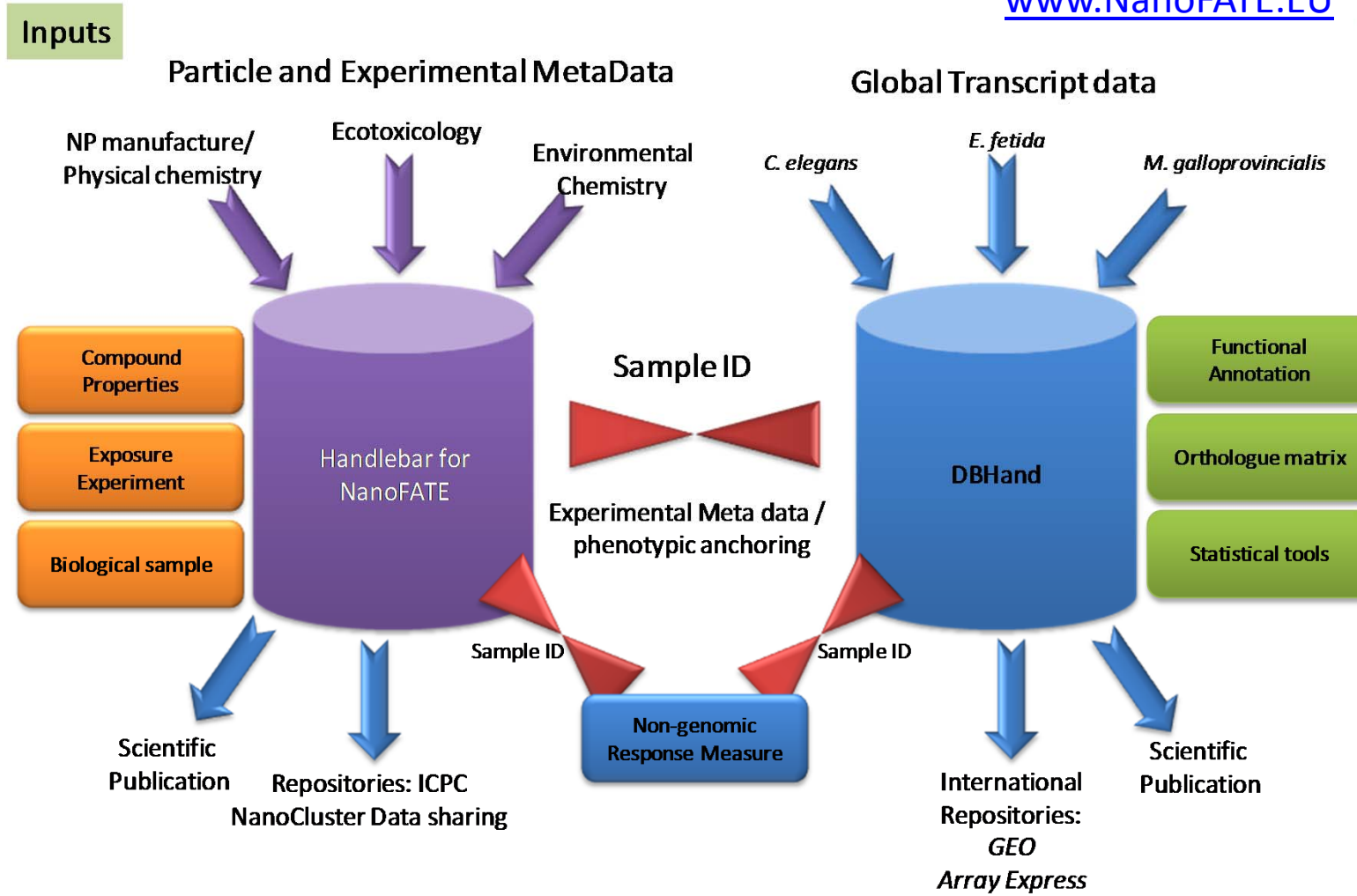
- + 0 Related Information
- + 1 General Information
- + 2 Classification and Labelling
- + 3 Manufacture, use and exposure
- + 4 Physical and chemical properties
- + 5 Environmental fate and pathways
- + 6 Ecotoxicological Information
- + 7 Toxicological information
- + 8 Analytical methods
- + 9 Residues in food and feedingstuffs
- + 10 Effectiveness against target organisms
- + 11 Guidance on safe use
- + 12 Literature search
- + 13 Assessment Reports

The NANOhub builds on  
OECD Harmonised Templates



<http://www.napira.eu/>

# Linking multiple meta-data with effects data





<http://nhecd.jrc.>



Intelligent search enables you to search for exact data taken from the results of all experiments described in the corpus articles.

NHECD IE extracts, from every scientific paper gathered by the NHECD crawler, a comprehensive, full and precise list of relations.

The information extraction system expected results include the following entities or relations:

- (1) Nano particle,
- (2) Model – Cell model or animal,
- (3) Attributes – NP size, Zeta potential, animal age, etc, and
- (4) Experiment attributes – mode of exposure, measurement assay etc.



# Acquisition, evaluation and public-oriented presentation of society-relevant data and findings relating to nanomaterials (DaNa)

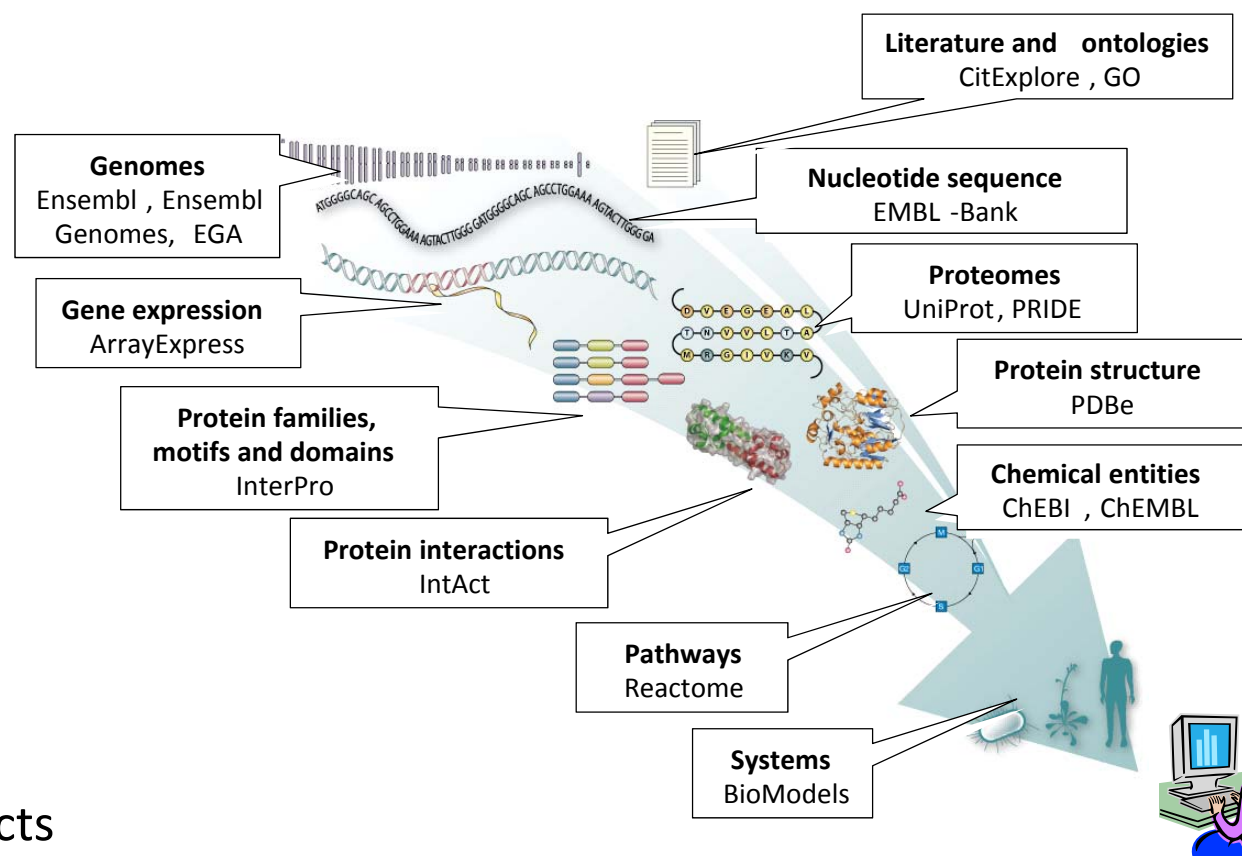
Contains information about products and applications with nanomaterials.  
Select an application or a material.

<http://nanopartikel.info/cms/Wissensbasis>





- Life sciences
- Medicine
- Agriculture
- Pharmaceuticals
- Biotechnology
- Environment
- Bio-fuels
- Cosmeceuticals
- Neutraceuticals
- Consumer products
- Personal genomes
- Etc...



# Recommendations



- Interface for daily capture of live data
  - => electronic notebook / new technologies (ipads/smart phones).
  - => Integrate with labview?
- Gateway to import data from existing databases.
- Ensure final database solution captures primary data (images, raw files etc.) not just processed results such as mean particle size, polydispersity index, LC<sub>50</sub> etc.
- Stakeholder workshop with students / postdocs & watch how they interact with proposed system
  - => Users will ultimately determine its success or failure.

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