US EU Roadmap
- Nanoinformatics-

Concept and Outline

Andrea Haase
Federal Institute for Risk Assessment (BfR)
Berlin, Germany
September 14th 2016
andrea.haase@bfr.bund.de

What is nanoinformatics?

Definition

Nanoinformatics is a **systematic methodology**
to **collect, organize, validate, store, share, model**, and **analyze data**
involved with nanotechnology processes and **materials**
for the **purpose** of **extracting useful information relevant to the nanoscale science** and **engineering** communities.

Computational nanoscience, conceived as falling within the broader term nanoinformatics, **includes** the **development** and **application of the critical tools** needed **for simulations, computations, and predictive modeling of nanomaterials, nanoscale devices, and nanosystems.**

According to US nanoinformatics roadmap, 2011

Objectives

Objective 1: vehicle for community interaction & resource to support different stakeholders

Why?
- high amount of money has been spent on nanoEHS so far, future resources are limited
- many different stakeholders (industries, academia, agencies etc.), each with its own objectives & needs

Thus, the nanoEHS community needs

1) to make highest possible use of the currently existing data
2) guidance on which type of research/ which type of data is needed in future
3) a medium to help the community to "self-assemble" & to get to know the different players, their tools as well as their individual needs/ objectives

What?
The nanoinformatics roadmap will support the community to
1) get to know the different stakeholders with their objectives
2) create a benefit for each
3) describe the nanoinformatics processes and tools
4) give an overview which tools are available to whom & how to use them
5) clearly describe the benefits of nanoinformatics at different phases of experimental work (experimental design, material prioritization & selection, identification of benchmarks, databases, data curation, data analysis, data sharing etc.)

Make the point clear that nanoinformatics is not only useful for some specialized experts but it is useful for all stakeholders!

Objectives

Objective 2: **capture, preserve, disseminate all publicly-available NM measurement data (experimental and computational)**

Why:
- avoids remeasurement
- provides access to previous measurements
- assures consistency in reporting of results
- facilitates planning new measurements
- keeps results secure
- increases the ROI for measurement support

What:
- build and link repositories
- ensure all publicly-funded nanomaterials measurement results are deposited

Certainly, this goal is big and a huge challenge.

However, the roadmap
- can raise public awareness of the benefits
- can describe how to achieve this goal step- by- step
- and explain what kind of infrastructure is needed for this

Objectives

Objective 3: Take advantage of existing NM measurement results

Why:
- To advance nanotechnology and expedite its commercialization
- To help different stakeholders to reach their specific objectives

What:
- Develop understanding of results
- Support model development
- Predict properties and performance of nanomaterials
- Correlate results with nanomaterial characteristics
- Correlate results with other functionality
- Advance development of new nanomaterials
- Support Safe-by-Design
- Support decision making
- Support regulation

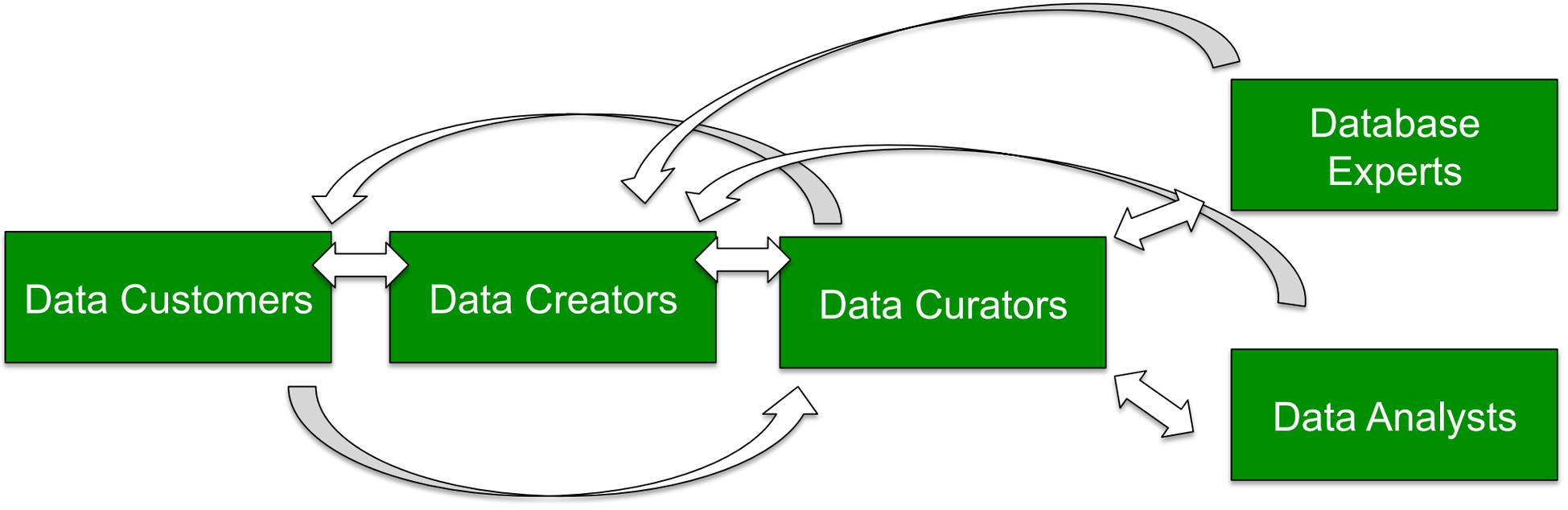
.... and many more

This objective is tightly linked to objective 2.

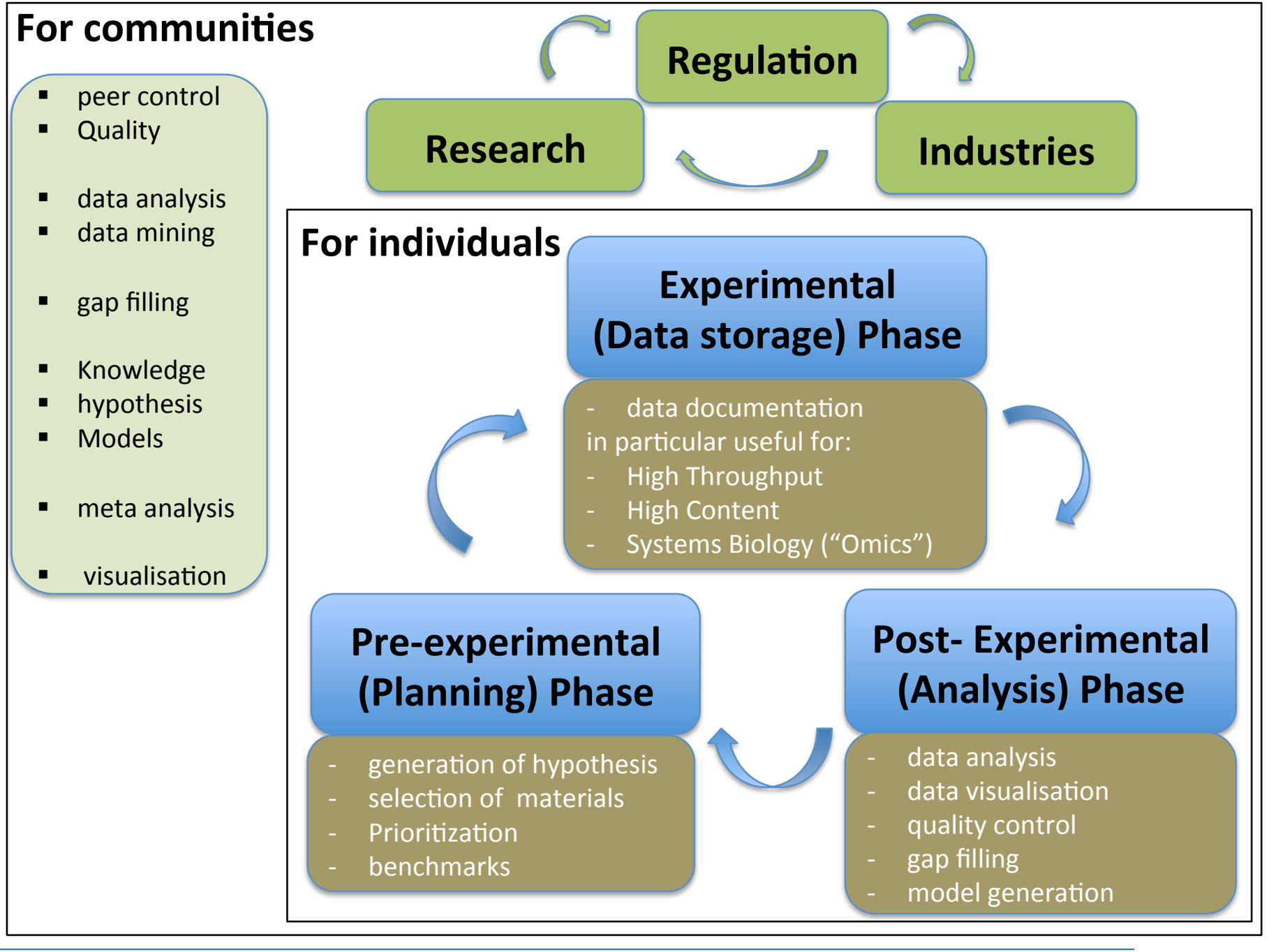
Objective 4: Identify specific pilot projects to reach the first three objectives. Describe the way forward (= roadmap)

Nanoinformatics “Players”

...not yet complete...



Nanoinformatics Processes and Impact



Short Outline

Section 1: Data Gathering and Data storage

a) Quality of Data
b) Data curation
c) Databases: ontologies, requirements, standards
d) metadata
e) Challenges: e.g. missing standards, heterogeneous datasets

Section 2: Data Analysis

a) **Material modelling**
- Modelling physical/ chemical descriptors of NM
- Explore how NM descriptors depend on the underlying physics and chemistry

b) **Chemoinformatics**
- Similarity Analysis
- Gap Filling (e.g. Read Across, QSAR)
- For exposure assessment & exposure modelling
- PBPK

c) **Bioinformatics** & AOP‘s

d) Guidance for other communities
- for pre-experimental planning, data storage, data analysis etc.
- challenges
- explain possible benefits and applications for different stakeholders (e.g. academia, regulatory agencies, industry)

Section 3: Data Accessibility & Data Exchange

Standards for information exchange

Section 4: Current Network

Overview on most important projects ongoing projects in EU and US

Training possibilities

Workshop and conference series

Section 5: Roadmap

Short term projects or action points

Medium term projects

Long Term projects (up to 2030)

Key Team (not complete)

Name		Affiliation
Andrea Haase	EU	**German Federal Institute for Risk Assessment (BfR)**
Frederick Klaessig	US	**Pennsylvania Bio Nano Systems**
Stephanie Morris, Mervi Heiskanen, Christina Liu	US	**NCI/ NIH**
Sabina Halappanavar	CAN	**Health Canada**
Mark D. Hoover	US	**US NIOSH**
Tomasz Puzyn	EU	**University of Gdansk**
Lisa Friedersdorf	US	**US NNO**
Treye Thomas	US	**US CPSC**
Anil Patri	US	**US FDA**
Stacey Stanridge	US	**US NNCC**
Christine Hendren	US	**Duke CEINT**
Nina Jeliazkova	EU	**IDEA**
Barry Hardy, Lucian Farcal	EU	**Douglas Connect**
Teresa Fernandes	EU	**Herriot Watts Uni Edingburgh**
Philip Doganis	EU	**Athens University**
Bengt Fadeel	EU	**Karolinska Institute**
Hubert Rauscher	EC	**JRC**
Pietro Asinari	EU	**Politecnico di Torino & European Materials Modelling Council**
Claus Svedson, David Spurgeon	EU	**NERC-CEH**
Eva Valsami- Jones, Iseult Lynch	EU	**Uni Birmingham**