EU-US nanoEHS Activities

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Overview

- Left EU-US workshop with one plan for the database and computational methods community of research (CoR);

- Nanoinformatics 2020 Roadmap is taking priority;

- Intend to use the earlier 'plan' as one basis for Roadmap; and

- Have begun reaching out for more resources

June 2016 Plan

- Based on workshop breakout discussion
- Use compilation of 'OECD' data by NANoREG to examine data completeness for some selected parameters in read-across.
- Mainly science, but with regulatory overtones;
- Important dates: 9/1/16 for data submission; 10/14/16 Open Tox milestone and mid-November for NANoREG meeting at OECD

Nanoinformatics 2020 Roadmap

- Raised at June workshop by Andrea Haase;
- Combines US report from 2011 with European activities;
- Teleconferences on outline in June and July;
- Mark, Mervi, Stephanie, Christine and I from the nanoWG; and
- My role is Andrea's 'point person' as co-chair of DB & CM CoR

Roadmap's Purposes

- US actions responsive to stakeholders
- EU actions more directed
  - Requested by EC with mid-2017 deadline
  - Core team identified
  - Draft could be made available shortly
  - Would be the basis for EU funding beyond 2018
  - Some co-funding possible
- Many aspects rely on Nanosafety cluster WG 4 and nanoWG for progress

Outline

- Intro
- Data Gathering and Data Storage
- Data Analysis
  - Material Modelling
  - Nanochemoinformatics
  - Bionanoinformatics
  - Guidance for other communities
- Data accessibility & Data Exchange
- Network/Stakeholders
- Roadmap

Worthwhile but concerns #1

- Quasi-NSF purpose – **role of stakeholders ?**
  - NSF: workshop leads up to funding
  - EU: roadmap leads up to funding
- No roadmap details and they may be pertinent
- Regulation mentioned and roadmap is science
  - Read across appears to be the prime objective
- Chapters (titles and descriptions) do not currently align with scientific disciplines/CoR's

Worthwhile but concerns #2

- Particle description not clear
  - Recommended explicit NPO & e-Nanomapper discussion separate from models.
- We will have many models in the future
  - Type 3 and 4 errors; validation; weather models
  - Recommended explicit discussion of uncertainty
- Terms and intent difficult to interpret
  - Descriptors & nano-descriptors (input variables & model output; computed property & measured property)

Worthwhile but concerns #3

- Chemoinformatics
  - Usually molecules and pharma; here grouping
  - Not normally environmental dispersal
  - Outline refers to exposure, hazard & PBPK
  - EPA exposure ontology suggested to demarcate
- Bioinformatics
  - Usually biological response
  - Here toxicity mechanism, adverse outcomes, systems biology

Worthwhile

- Opportunity to communicate across many disciplines;

- Opportunity to set groundwork for *in silico* models, including uncertainty distributions, validation, relationship to measurements;

- Opportunity to set a path from material to exposure to toxicity paralleling the path from material to performance to commercialization.

- Opportunity for nanoWG & WG4 teamwork

FK Actions

- Making a list of people who might be interested and contacting them (25/8/4).

- Communicating activity across stakeholders (academia, industry, NGOs).

- Informal comments sent to Andrea.

- Preparing for 10/24 meeting

- My 10/24 part will focus on NANoREG data for OECD materials using zeta potential & the JRC template to read across.