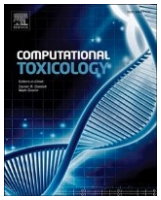
Computational Toxicology 30 (2024) 100316

Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.sciencedirect.com/journal/computational-toxicology



Short Communication

NNI nanoinformatics conference 2023: Movement toward a common infrastructure for federal nanoEHS data computational toxicology: Short communication

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Abbreviations: AOP-DB, Adverse Outcome Pathway Database; API, Application Processing Interface; CARE, Collective Benefit, Authority to Control, Responsibility, and Ethics; COR, Communities of Research; CPSC, Consumer Product Safety Commission; DIIG, Database and Informatics Interest Group; ENM, Engineered nanomaterial; EPA, Environmental Protection Agency; EU, European Union; FAIR, Findable, Accessible, Interoperable, and Re-usable; FDA, US Food and Drug Administration; ICP-MS, inductively coupled plasma mass spectrometry; InChI, International Chemical Identifier; ISA-TAB-Nano, Investigation/Study/Assay (ISA) tab-delimited (TAB) format, specifically for Nanomaterials data; IUPAC, International Union of Pure and Applied; NIOSH, National Institute for Occupational Safety and Health, USCDC; NInChI, InChI for Nano; NLP, Natural Language Processing; NM, Nanomaterial; NNI, US National Nanotechnology Initiative; NNCO, US National Nanotechnology Coordination Office; nanoEHS, nano Environmental, Health and Safety; OSHA, Occupational Safety and Health Administration; OSTP, US Office of Science and Technology Policy; RDF, Resource Description Framework; SSbD, Safety and Sustainability by Design; TRUST, Transparency, Responsibility, User focus, Sustainability and Technology; U.S, United States.

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https://doi.org/10.1016/j.comtox.2024.100316 Received 25 April 2024; Accepted 15 May 2024

Available online 16 May 2024

2468-1113/Published by Elsevier B.V.

ARTICLEINFO

ABSTRACT

Keywords: The National Nanotechnology Initiative organized a Nanoinformatics Conference in the 2023 Biden-Harris AdNanomaterials ministration's Year of Open Science, which included interested U.S. and EU stakeholders, and preceded the U.S.- Emerging materials EU COR meeting on November 15th, 2023 in Washington, D.C. Progress in the development of a common

Safe/sustainable by design Database Interoperability nanoinformatics infrastructure in the European Union and United States were discussed. Development of contributing, individual

database projects, and their strengths and weaknesses, were highlighted. RecommenInfrastructure dations and next steps for a U.S. nanoEHS common infrastructure were discussed in light of the pending update FAIR of the National Nanotechnology Initiative (NNI)'s Environmental, Health and Safety Research Strategy, and U.S. efforts to curate and house nano Environmental Health and Safety (nanoEHS) data from U.S. federal stakeholder groups. Improved data standards, for reporting and storage have been identified as areas where concerted efforts could most benefit initially. Areas that were not addressed at the conference, but that are critical to progress of the U.S. federal consortium effort are the evaluation of data formats according to use and sustainability measures; modeler and end user, including risk-assessor and regulator perspectives; a need for a community forum or shared data location that is not hosted by any individual U.S. federal agency, and is accessible to the public; as well as emerging needs for integration with new data types such as micro and nano plastics, and interoperability with other data and meta-data, such as adverse outcome pathway information. Future progress will depend on continued interaction of the U.S. and EU CORs, stakeholders and partners in the continued development goals for shared or interoperable infrastructure for nanoEHS.

1. Introduction

With the pending update of the National Nanotechnology Initiative (NNI)'s Environmental, Health and Safety Research Strategy [3] there is an impetus to review the core areas identified in 2011 to spotlight specific areas of progress and change across the diverse nano environmental health and safety (nanoEHS) research area, and to identify areas of high relevance and remaining unmet needs. These encompass both scientific developments and broader societal considerations. Informatics was identified as a cross-cutting theme that would enable and integrate the six individual research areas.

Since 2011, many individual efforts aimed at improving the existing nanoEHS research infrastructure have been initiated, both in the United States with NNI member agencies, and through many efforts in the European Union. These efforts, though not concerted, are seen to be moving toward infrastructure development through database and tool creation, interoperated via application programming interfaces, to address pertinent questions that have arisen in the last decade. The NNI member agencies have created the Database and Informatics Interest Group (DIIG) to address the plethora of databases and tools created to address agency issues pertaining to emerging materials, specifically nanoEHS related, and to determine a path forward for data accessibility, integration, and sustainability for nanoEHS data among U.S. federal partners. The NNI member agencies are aware of the progress made in this area by EU partners and are also concerned to keep pace with these efforts with an eye toward U.S.-EU data interoperability in the future. NNI member agencies agree in the shared requirement for global alignment to foster reuse of regulatory relevant data in a global market. These interests and concerns have motivated the recent focus on this topic at the first NNI's 2023 Nanoinformatics Conference, which was coordinated as part of the NNI U.S.-EU Communities of research (CORs) meeting.

1.1. Background

Recent efforts of the NNI DIIG have focused on the creation of a federal nanoEHS consortium, which includes U.S. federal partners (EPA, NIOSH, OSHA, CPSC, FDA) with the primary goal of developing data standards consistent with FAIR (Findable, Accessible, Interoperable and Reusable) principles [4,5]. Consortium partners have recently exchanged datasets, which do not include proprietary or security limitations. These "test" data consist of relational database structures or tables that are contributed by each partner agency for processing and curation. A focus on data interoperability and sustainability of hosting is a secondary goal of this effort. The Environmental Protection Agency (EPA) has developed the OntoSearcher tool to expedite this process, which partially automates the ontology mapping process thereby reducing onerous manual curation [6]. Through this U.S. federal consortium effort, and the coordinated curation and semantic integration of the individual datasets, member agencies hope to improve the data standards and interoperability of individual nanoEHS datasets. Two unresolved issues are 1. a location for data hosting that is both sustainable long-term and decentralized; and 2. whether semantic mapping will provide a useful format in the long term that justifies the effort required to implement it and if this approach meets the needs of various stakeholders, especially of non-technical users.

2. Conference overview

The National Nanotechnology Coordination Office (NNCO), on behalf of the U.S. government's National Nanotechnology Initiative (NNI; https://www.nano.gov/national-nanotechnology-initiative), in conjunction with the EPA and co-hosted by Duke University's InFRAMES (https://inframes.pratt.duke.edu/), coordinated the recent NNI's Nanoinformatics Conference; https://www.nano.gov/NNINanoinformaticsConference, an in-person-only event on November 15th in Washington, D.C. Government, industry and academic experts in computer science, cybersecurity, informatics, and nanoEHS and risk assessment came together in the 2023 Biden-Harris Administration's Year of Open Science to discuss how to address data challenges with the Data Informatics Interest Group of the NNI federal consortium for nanoEHS data and to determine how and where federal partners can best maintain, store and integrate their respective federal nano-related datasets to promote data sharing and longevity between partners in the United States and internationally. The conference was motivated by current activity in the informatics research area, and progress in the area of nanoinformatics described in two documents, the U.S.-EU Roadmap effort [1] and the NNI Environmental Health and Safety Research Strategy: 2024 Update [3,7]. Both documents identified two main needs in the areas of nanoinformatics to be the lack of sufficiently accessible data for model development and the lack of a much-needed community infrastructure to support data and model accessibility and promote standards for metadata reporting and interoperability.

The Nanoinformatics Conference preceded the U.S.-EU COR (https://us-eu.org/) meeting. The NanoEHS CORs are seven individual communities of researchers from government, academia, and industry, originally formed in 2011 to address questions about the potential environmental, health, and safety (EHS) implications of nanomaterials. The Database and Computational Modeling for NanoEHS COR is currently co-chaired by Fred Klaessig (United States) and Thomas Exner (European Union). The NNCO, on behalf of the NNI, provided technical and administrative support for the Nanoinformatics Conference, and was the federal government point of contact for both the Nanoinformatics Conference and the U.S.-EU NanoEHS COR meetings. The conference was co-chaired by Dr. Holly Mortensen of EPA's Center for Public Health and Environmental Assessment in the Office of Research and Development, and Jaleesia Amos, a Doctoral Candidate from Duke University Pratt School of Engineering.

2.1. Keynote presentations

Two keynote presentations were made by Professor Stacey Harper of Oregon State University, College of Agricultural Sciences and College of Engineering, and Dr. Christopher Marcum, Senior Statistician and Senior Scientist in the Office of the Chief Statistician of the United States at the White House Office of Management and Budget, previously the Assistant Director for

Open Science and Data Policy in the White House Office of Science and Technology Policy (OSTP). Dr. Harper gave a broad overview of the field of nanoinformatics, focusing on the "What and Why of Informatics. Dr. Harper outlined the interdisciplinary fields of computer science, information systems, and their intersection with data science, and human–computer interactions. She underlined the issues surrounding data collection, storage, and limitations to processing and analyses that are pervasive to nanoinformatics research at this time. Dr. Harper also invited the audience to understand the connections between informatic efforts and improvement in data security and quality of life, citing diverse examples from healthcare, social media, and smart public services. Dr. Marcum inspired the audience by giving insight into the Biden-Harris Administration actions to advance open science throughout 2023 as a *Year of Open Science*; (https://www.whitehouse.go v/ostp/news-updates/2024/01/31/fact-sheet-biden-harris-admini stration-marks-the-anniversary-of-ostps-year-of-open-science/), defined as "*the principle and practice of making research products and processes available to all, while respecting diverse cultures, maintaining security and privacy, and fostering collaborations, reproducibility, and equity*". Dr. Marcum underlined the importance of open science and public access to data as priorities of the Biden-Harris Administration that support innovation and enterprise, while underlining that federal data falls on a continuum from completely closed to completely open-with appropriate controls along the continuum for increasing public access to federal data, including confidential statistical data (https://www.statspolicy.go v/). Dr. Marcum also highlighted OSTP's partnership with challenge.gov that engaged researchers, community scientists, educators, innovators, and the broader public to highlight efforts to expand access to research for the benefit of science and society (https://www.whitehouse.gov/ost p/news-updates/2024/03/21/white-house-office-of-science-technolo gy-policy-announces-year-of-open-science-recognition-challenge- winners/).

2.2. Conference presentations

The conference presentations were led by Dr. Fred Klaessig (Pennsylvania BioNano Systems), who provided highlights of the many Roadmapping and research program efforts, mostly EU-focused; e.g., the Closer to the Market Roadmap [8]; the Regulatory Research Roadmap (https://www.nanosafetycluster.eu/nsc-research-regulatory-road map-2017/); Responsible Research & Innovation [9]; FAIR/TRUST Initiatives and the AOP-Wiki, JRC Repository of commercial benchmark materials (from Europe) (https://joint-research-centre.ec.europa. eu/scientific-tools-and-databases/jrc-nanomaterials-repository_en), and database efforts such as the NANoREG instance of eNanoMapper. Dr. Klaessig focused on data collection and curation, including workflow and database management best practice as proposed by Haase and Klaessig [1], and underlined the importance of annotation and federated databases.

This topic was continued by Dr. Thomas Exner of Seven Past Nine, in his presentation discussing knowledge management and the implementation of "FAIR Data Standards for Nanomaterials and Nanotechnology". Dr. Exner noted a potential issue with storing of data in (structured or unstructured) databases that may provide a structure that is not necessarily useful for its re-use and modeling. While especially regulatory databases are focusing on specific materials, large sets of data on a specific endpoint for multiple materials are critical for nanosafety model development to reduce reliance on animal testing for both ethical and cost reasons. This move away from animal testing toward *in silico* methods provides a major driver for adoption and implementation of FAIR data standards focusing on data re-use and data sharing. Dr. Exner explained the principles of TRUST (**T**ransparency, **R**esponsibility, **U**ser focus, **S**ustainability and **T**echnology for data repositories) [10], CARE (Collective Benefit, Authority to Control, Responsibility, and Ethics as first proposed for management of indigenous data) [11], and AI- readiness in the EU [12], which need to be followed, besides FAIR, to establish a data sharing and reusing mentality essential for addressing data needs for what is referred to in the EU as Safety Assessment, Safe By Design (SbD) and more recently Safe and Sustainable by Design (SSbD). Dr. Exner discussed the much-needed community standards for nanomaterials data [13,14], with a harmonized presentation format for data, but also the need for a "distributed data lake", where archetypes and templates can assist in storage and harmonization of very diverse data and transforming it into input for models.

Dr. Holly Mortensen, outlined the efforts of the EPA, in conjunction with other U.S. and EU partners to establish community-driven best practices, and support common infrastructure to connect data resources. Dr. Mortensen highlighted recent EPA efforts with NaKnowBase [15] and ongoing work to address the interoperability of U.S. federal agency nanomaterials data [6] semantic mapping efforts that leverage existing ontologies in order to break down federal data silos and promote FAIR data standards for nanoEHS. Dr. Mortensen discussed what she referred to as the "nomenclature debacle" for nanomaterials, EPA's efforts to use Natural Language Processing (NLP) to develop and EPA-specific nomenclature for nanoEHS, and the lack of utility of ISA-TAB-Nano [16] in meeting current data storage and interoperability needs. She introduced the concept of graph databases, specifically the Resource Description Framework (RDF), and how this format may address heterogeneity and interpolation issues inherent to nano data. Dr. Mortensen introduced the RDF mapping of the EPA Adverse Outcome Pathway Database (AOP-DB) [15] and the EPA NaKnowBase, and the EPA Ontosearcher tool, [6]; https://catalog.data.gov/dataset/naknowba se-interoperability-tools. She discussed these semantic mapping efforts and tools in relation to the collaborative efforts of the NNI DIG, and agency partners to implement the use of these EPA tools to expedite processing, and manual curation, and move toward a shared data environment. Finally, Dr. Mortensen challenged the group for their opinions on this process and specific formats for the integration and sharing of data across U.S. and international efforts.

Dr. Vladimir Lobaskin, of the University College Dublin presented lessons learned from four recent EU-funded nanoinformatics projects, NanoSolveIT, NanoCommons, NanoInformaTIX, and eNanomapper, that have largely followed the directions outlined by The EU-U.S. Nanoinformatics Roadmap 2030 and formed the backbone of the European nanoinformatics effort. These projects have delivered frameworks for nanomaterial data management: data collection templates, ontologies, databases, data processing and modeling tools, which were integrated into public knowledgebases to ensure the data FAIRness. The goals presented by Dr. Lobaskin, representative of that period in the European Union, were to understand health and environmental risks posed by enginered nanomaterials (ENM), to identify material properties determining their functionality, toxicity, and sustainability, and to eliminate or reduce the associated risks. This effort reduced the need for animal testing, making materials SSbD. Dr. Lobaskin also underlined the essential nanoinformatics needs identified by these projects: (i) standardization and automation of data collection and management, (ii) development of a modeling framework that allows for prediction of functionality and hazard from the material properties using quantitative structure–activity relationships, (iii) the need to develop nano-specific mechanism-aware predictive schemes such as the Adverse Outcome Pathway (AOP) framework and other framework or concept because of the higher complexity of NM compared to chemicals and bulk materials, facilitated by (iv) provision of advanced ENM descriptors and characterizations that reflect the features responsible for their activities and functionalities. In the next funding period, as outlined in the Horizon Europe framework program, the European Union aims to establish a European Materials Platform to facilitate SSbD principles.

Dr. Kenneth Flores discussed informatics and modeling needs in the context of drinking water applications, specifically for nanomaterial standards and screening protocols for water purification. Nano-enabled technologies for water treatment are promising but there is a need for risk evaluation of leaching of insoluble nanomaterials as well as dissolved metals. Point of use (POU) systems are increasing in use, but the National Sanitation Foundation has expressed a need for effective protocols for quantification and discrimination between dissolved and nanoparticulate metals in drinking water matrices. Dr. Flores presented the agreement of results from an interlaboratory screening method utilizing centrifugal ultrafiltration with inductively coupled plasma mass spectrometry (ICP-MS) as a mode of detection, from three independent university laboratories, in collaboration

with NSF. Results from the study found accurate discrimination between dissolved and nanoparticulate species in the µg/L concentration range, for various mixtures of nanoparticulate and dissolved gold species, resulting in <10 % error. In addition, temporal variability was evaluated in terms of effect on NM quantification and discrimination. More in depth details of this interlaboratory study can be found in the recently published work. (https://doi.org/10.1016/j.scitotenv.2023.168686).

Dr. Marvin Martens presented his work with the semantic web applications, and described the potential of RDF in seamlessly integrating data from separate databases and disparate data sources. Through examples drawn from AOP-Wiki, [17], the EPA AOP-DB [18], and Nanosafety [19] and WikiPathways data [20], Dr. Martens demonstrated the interoperability achievable through this methodology. The presentation sparked a discussion on the accessibility and usability of these techniques to non-technical communities.

Prof. Iseult Lynch, of the University of Birmingham, discussed progress towards implementation of a nano-specific chemical identifier that builds on and extends the standard International Union of Pure and Applied (IUPAC) international chemical Identifier (InChI), called the InChI for Nano or NInChI [21], as a way to standardize nanomaterial nomenclature. Since the original prototype was developed, an international consortium has been working on developing the formal standard in collaboration with the InChI Trust, and testing it against a wide range of nanomaterials of increasing compositional and structural complexity. Implementation of NInChI will facilitate integration of nanoEHS datasets by increasing confidence in the materials similarity and provenance across datasets.

Closing discussion focused on risk assessment and regulatory needs, led by EPA Senior Scientist Annie Jarabek. Ms. Jarabek focused on illustrating issues of assessment for inhalation effects of air pollution, wildfires, and 3-D plastics printing; highlighting the role of inhalation particle dosimetry modeling to translate exposure to internal dose metrics. She noted that emerging appreciation and understanding of the effects of ultrafine particles in the air pollution arena is one that overlaps and would be mutually beneficial for collaboration with the nano community. Risk assessment is moving to comprehensive source to outcome modeling [22]. An ongoing National Institute for Environmental and Health Sciences (NIEHS) Environmental Health Language Collaborative's use case for particulate matter less than 2.5micrometers or smaller (PM2.5) and asthma https://www.niehs.nih.gov/research /programs/ehlc/use-cases/bio) was given as an example of an attempt to develop semantic modeling language to support the entire continuum from exposure to adverse outcome. Ultimately, quantitative AOPs (qAOPs) are needed in regulatory applications [23]. Ms. Jarabek emphasized the need for modularity and interoperability along this continuum as many measurements or results relevant to risk assessment already represent standard parameters or outputs from various models. Articulation of assumptions and policies are critical in any assessment workflow. She emphasized both FAIR reporting standards and the complimentary TRUST principles [10] to ensure stakeholders regarding data integrity for use in risk assessment.

3. Conclusions and conference outcomes

Audience discussion ensued enthusiastically throughout and during the sessions. Concern was expressed for the ability to maintain databases, management, and financial support, longevity of individual efforts and the effect this has on trust and perception of data quality. Successful EU nano projects were highlighted, whereby coordinated and well-funded government projects have clearly had an impact on data infrastructure and integration in the European Union. The successful implementation of the U.S.-EU Roadmap for nanoinformatics and nanoEHS, as described in [1] in the United States is dependent on the continued progress and development of U.S. federal consortium effort. Data types contributed by each agency do not constitute special handling or security measures, though these types of data exist but are purposefully not included in this effort. Improved data standards, for reporting and storage have been identified as areas where concerted efforts could most benefit initially. A separate manuscript describing the U.S. federal consortium's process of data curation, processing for semantic integration, and analyses to assess the variability across datasets is currently in preparation. Areas that were not addressed at the conference, but that are critical to progress of the U.S. federal consortium effort are the evaluation of data formats according to use and sustainability measures; modeler and end user, including risk-assessor and regulator perspectives; a need for a community forum or shared data location that is not hosted by any individual U.S. federal agency, and is accessible to the public; as well as emerging needs for integration with new data types such as micro and nano plastics, and interoperability with other data and meta-data, such as adverse outcome pathway information. As illustrated in the graphical abstract, the flow of data envisioned in the US-EU Nanoinformatics 2030 Roadmap effort, the "Virtual" data integration described by Maier [2], and the current conceptual model of individual U.S. agency database contributions, each contribute to the process of global alignment and harmonization of nanoEHS data across US-EU communities. Future progress will depend on continued interaction of the U.S. and EU CORs, stakeholders and partners in the continued development goals for shared or interoperable infrastructure for nanoEHS.

CRediT authorship contribution statement

Holly M. Mortensen: Conceptualization, Project administration, Supervision, Writing – original draft, Writing – review & editing. **Jaleesia D. Amos:** Project administration, Writing – review & editing. **Thomas E. Exner:** Writing – review & editing. **Kenneth Flores:** Writing – review & editing. **Stacey Harper:** Writing – review & editing. **Annie M. Jarabek:** Writing – review & editing. **Fred Klaessig:** Writing – review & editing. **Vladimir Lobaskin:** Writing – review & editing. **Iseult Lynch:** Writing – review & editing. **Christopher S. Marcum:** Writing – review & editing. **Marvin Martens:** Writing – review & editing. **Branden Brough:** Project administration. **Quinn Spadola:** Project administration. **Rhema Bjorkland:** Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgments

The authors would like to acknowledge the NNI NEHI DIIG partners, and federal organizing committee members, specifically Keana Scott (NIST), Treye Thomas (CPSC), Jay Vietas (NIOSH), Anil Patri (FDA), Natalia Garcia Reyero Vinas (DOD OSD), Kanakadudurga Addepalli (NIH), Charles Schmitt (NIH), Nora Savage NSF), and Luisa Russell (NIH) for their participation and organization of the event. The authors would also like to thank Geoff Holdridge (contractor NNCO) and Mark Weisner (Duke University) as well as U.S. and EU participants for their contributed views and discussion that ultimately led to the opinions and goals set out in the current manuscript, as well as Adam Biales and Michael F. Hughes of the EPA, and reviewers in the Office of Science and Technology Policy (OSTP), for their careful review and comments on the manuscript.

Disclaimer

These proceedings are a product of contributions from federal and non-federal authors. As such, views expressed by non-federal participants do not represent views or policies of federal agencies.

Funding

Funding for the 2023 Nanoinformatics Conference in Washington, D. C. was provided by the U.S. government's National Nanotechnology Initiative (NNI). Supplemental travel funding for JDA and AMJ were provided by Duke University's INFRAMES program. TEE and IL acknowledge the EU Horizon Europe funded project WorldFAIR (Grant Agreement No. 101058393) and Innovate UK for funding UoB participation in WorldFAIR (Grant No. 1831977).

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