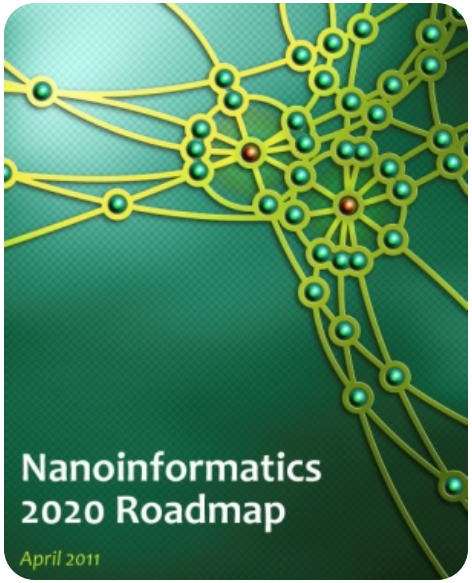
Nanoinformatics

A series of workshops by the broad nanoinformatics community

- 2007 Exploratory Nanoinformatics meeting
- 2009 Nanomanufacturing Summit Panel
- Nanoinformatics 2010
- Nanoinformatics 2020 Roadmap Published (April 2011)
- Nanoinformatics 2011: Q-SARs and MinChar
- Nanoinformatics 2012 Summer Workshop: Tools and Resources
- Nanoinformatics 2013: Informatics for Nanomanufacturing
- Nanoinformatics 2015: Enabling Successful Discovery & Applications



DATA – TOOLS - SHARING

Nanoinformatics 2015

"Enabling Successful Discovery and Applications"

NNN Workshop: January 26-28, 2015; Arlington VA

- **Nanoinformatics Tutorial**
- Session 1: Purpose-driven Nanoinformatics
- Session 2: Inventory of Nanoinformatics Data and Tools
- Session 3: Nanoinformatics for Design of Materials, Manufacturing, and Products
- Session 4: Nanoinformatics for Risk
- Poster Presentations and Discussion
- Session 5: Uncertainty Quantification and Informatics Robustness
- Session 6: Sharing and Conceptual Integration of Data Elements Across Resources
- **Nanoinformatics Charette**

http://nanoinformatics.org/2015/agenda

Tuominen, 3/19/2015

Nanoinformatics Tutorial

- Mark Tuominen – **"Broad introduction to science informatics and lab automation strategies"**
- Yoram Cohen – "**Assessing Environmental Impact Analysis**"
- Mark Hoover – "**ONAMI, NIL, Good Nano Guide, Nanomaterials Registry**"
- Gerhard Klimeck – "**nanoHub**"

- Covered some fundamentals and current status
- Generated discussions on overarching purpose and strategy

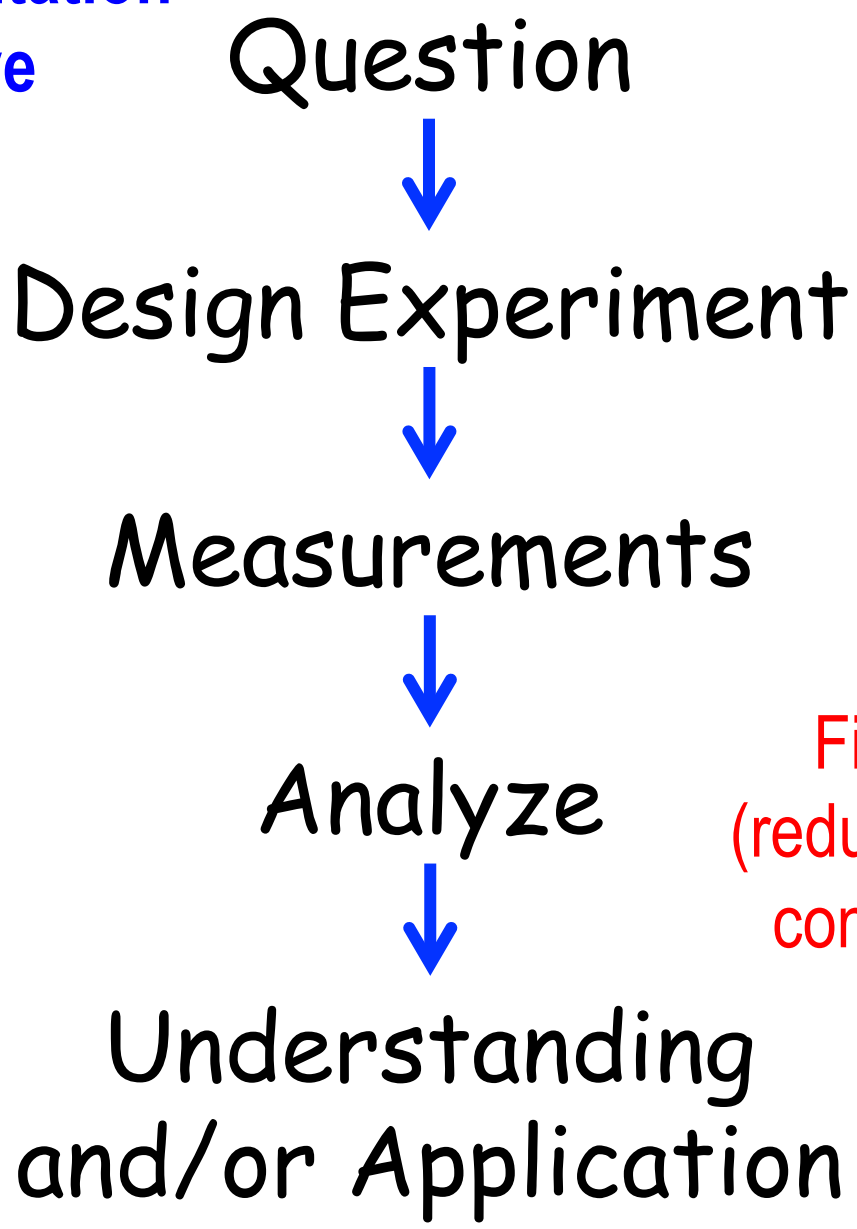
Science Informatics

Information Automatic

In the broadest sense, we try to—as much as currently possible—automate working with the information associated with science.

- To more broadly leverage the information already gathered.
- To reduce uncertainty and assist in decision-making
- To better automate processes that build science.
- To save time and money.
- To help assure safety for people and the environment.
- To build in greater intelligence into the entire system.

Experimentation Perspective



Curiosity, need

An attempt to address question

Acquiring data

Find trends, correlations (reduction); building models or connecting to existing ones

Sharing: service and value to society

Once in a while things actually work this way; the real world can be more convoluted.

Nanoinformatics

- the science and practice of determining which information is relevant to the nanoscale science and engineering community, and then developing and implementing effective mechanisms for collecting, validating, storing, sharing, analyzing, modeling and applying that information.

Nanoinformatics

Purpose? For understanding and application

Physical Properties

Applications Development

Modeling and Simulation

Materials

Engineering

Education

Manufacturing

EHS

Biological Interactions

Business

Important to recognize the different perspectives and agendas of diverse domains

Nanoinformatics

Workshop Agenda

A) Sessions 1-6: Presentations, discussion, and posters

- Keep in mind that this is a **multidisciplinary audience**
- Presenters should please clearly describe the **thematic purpose** of your project; the original intended domain of use
- Presenters, is your nanoinformatics output **currently available** for other users?
- Discuss **ways for greater or new impacts** are possible from your project, especially through some specific kinds of **collaboration** with others.
- Everyone, actively **identify opportunities** for expanding the real-world impact of nanoinformatics
  - By expanding the reach of existing projects
  - Through project-to-project cooperation
  - Through the creation of timely data/tools/methods -- for science, technology development, EHS, applications, or manufacturing.

B) Nanoinformatics Charrette

– strategically building potential opportunities into collaborative activities and projects; to inform the broader community of these ideas and activities and to welcome participation

Nanoinformatics

Session 1: Purpose-driven Nanoinformatics

8:00-8:10 Workshop Welcome and Purpose - Stacey Harper and Mark Tuominen

8:10-8:30 "**Federal Initiatives on Nanoinformatics**" - Lisa Friedersdorf (National Nanotechnology Coordination Office)

8:30-8:50 "**Data at NIST: Next Steps Toward Discoverability, Access, and Analysis**" - Robert Hanisch (NIST)

8:50-9:00 Discussion

Session 2: Inventory of Nanoinformatics Data and Tools

9:00-9:20 "**CEINT Nanoinformatics Knowledge Commons: Building research tools to meet the needs of the nano EHS research community**"- Greg Lowry (CEINT, Carnagie Mellon University)

9:20-9:40 "**The National Cancer Institute (NCI) Nanotechnology Working Group (Nano WG)**" - Mervi Heiskanen (NCI Nanotechnology Working Group)

9:40-10:00 "**nanoHUB.org: A Home for Scientific Exploration with Simulation Tools and Data Sets**" - Michael Zentner (nanoHub)

10:20-10:40 "**Uncertainty Quantification within nanoHub**" Alejandro Strachan (Purdue University)

10:40-11:00 "**Nanomaterials Registry**" - Tony Hickey (Nanomaterial Registry)

11:00-11:20 "**Nano Bibliometrics**" - Alan Porter (Georgia Institute of Technology)

11:20-11:40 "**caNanoLab: A collaborative nanomaterial data repository supporting cancer biomedical research**" - Stephanie Morris (NIH)

11:40-12:00 Discussion

Session 3: Nanoinformatics for Design of Materials, Manufacturing, and Products

1:00-1:20 "**Applying Informatics to Autonomy in Experimentation**" - Jason Poleski (Lockheed-Martin)

1:20-1:40 "**Materials informatics for the discovery and design of 2D materials**" - Richard Hennig (University of Florida)

1:40-2:00 "**Informatics for Combinatorial Materials Science**" - Ichiro Takeuchi (University of Maryland)

2:00-2:20 "**Process Modeling and Control in the Nanomanufacturing of 2 and 3-D Nanostructures using Directed Assembly of Nanoparticles**" - Ahmed Busnaina and Cihan Yilmaz (Northeastern)

2:20-2:40 "**Automatic Information Extraction of Experiments from Nanocrystal devices Development Papers**" - Masaharu YOSHIOKA, Thaer Dieb, Shinjiroh HARA (Hokkaido University Japan)

2:40-3:00 Discussion

Session 4: Nanoinformatics for Risk

3:20-3:40 "**Quantitative Structure-Activity Relationships for Engineered Nanomaterials: Advances and Challenges**" - Rong Liu and Yoram Cohen (UCLA)

3:40-4:00 "**Informatics Approaches to Advance Risk Estimation in Research, Design, Manufacture and EHS**" - Marty Fritts (NIST)

4:00-4:20 "**Evaluation of the Information Content in Proposed QSAR Descriptors via Machine Learning Meta-Analysis of In Vivo Nanotoxicity Experiments**" - Jeremy Gernand (Pennsylvania State University)

4:20-4:40 Discussion

Session 5: Uncertainty Quantification and Informatics Robustness

8:00-8:20 "**InterNano: Information Resources for Nanomanufacturing**" - Jeff Morse (InterNano, National Nanomanufacturing Network)

8:20-8:40 "**Nanoinfo.org: An Integrated Nanoinformatics Web-Portal**" - Dennis Bacsafra, Muhammad Bilal, Michelle Romero, Haven Liu, Rong Liu, and Yoram Cohen (UCLA)

8:40-9:00 "**Probabilistic Assessment of the Potential Environmental Impact of Engineered Nanomaterials**" - Muhammad Bilal, Haven Liu, Rong Liu, and Yoram Cohen (UCLA)

9:00-9:20 Discussion

Session 6: Sharing and Conceptual Integration of Data Elements Across Resources

9:20-9:40 "**Principles and a conceptual framework for functional data integration**" - Mark Hoover (CDC/NIOSH)

9:40-10:00 "**Towards a visual taxonomy of nanoparticles**" - Victor Maojo, (Universidad Politécnica de Madrid, Spain)

10:20-10:40 "**Increasing the Robustness of Nanoinformatics Resources: The CODATA-VAMAS Uniform Description System**" – Steven Freiman (CODATA, R&R Data Services)

10:40-11:00 "**Evaluation of the Potential Medical Effects of Engineered Nanomaterials in Army Systems**" - Mark Widder (US Army Center for Environmental Health Research)

11:00-11:20 Discussion

Charrette topic candidates:

- Efforts to *publicize and teach* the principle tenets of nanoinformatics

- **Indentify metrics of success for nanoinformatics** (usages, who, how many, how used, etc

- **Workflow – Streamlining the effort in nanoinformatics. Model systems of workflow.**

- **Possible new uses & new users of nanoinformatics tools.** Two-way sharing of methods and tools with people in other disciplines (eg MGI, synthetic bio, cloud manufacturing). Building literacy of science informatics. Ways to look across tools (including mapping ontology use-to-use.) Explicitly demonstrate tools to each other, including with companies who have tools or hope to develop tools. e.g., MGI-NKI two way efforts.

(blue – chosen for charrette discusssion)

Charrette topic candidates (continued):

- Mechanisms for better incorporation of unstructured information. (eg big data)
- Build a stronger set of tools and data to help advance materials and manufacturing informatics. (including metrological communications)
- Definitional efforts – building terms and definitions – helps to identify the field and its evolution over time. (eg caNanoLab efforts on term thesaurus)
- Metadata – minimum characteristics and beyond. (recognizing that min char metadata is a minimum essential for discoverability and searchability, but more detailed metadata is needed, and distinct for each field of activity, to well document the data provenance.)
- Emphasize and articulate the multidiscipline and multi-perspective aspect of nanoinformatics. It is a strength and advantage to explicitly recognize it and describe it. For example, research-focus vs application-focus vs political/sociological – representing different communities of interest/practice
- Framework for data management best practices. Articulation of the value proposition for doing this to help build stronger culture in doing research and development in a way that engenders quality data practices, with accessibility/ discoverability/searchability.

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