Nanoinformatics 2010:
A Collaborative Roadmapping and Planning Project

Holiday Inn National Airport
Arlington, VA
November 3 – 5, 2010

Nanoinformatics 2010 is a collaborative roadmapping and planning project at which informatics experts, nanotechnology researchers, and other stakeholders and potential contributors will jointly develop a roadmap for the area of nanoinformatics.

Nanoinformatics 2010 is designed to survey the landscape, generate a roadmap, and stimulate collaborative activities in the area of nanoinformatics. By doing so, it will accelerate the responsible development and use of nanotechnology. Workshop themes include:

- **Data:** Data Collection and Curation
- **Tools:** Tools for Innovation, Analysis, and Simulation
- **Sharing:** Data Accessibility and Information Sharing

Nanoinformatics involves the development of effective mechanisms for collecting, sharing, visualizing, modeling and analyzing information relevant to the nanoscale science and engineering community. It also involves the utilization of information and communication technologies to help launch and support efficient communities of practice. Nanoinformatics is necessary for comparative characterization of nanomaterials, for design and use of nanodevices and nanosystems, for instrumentation development and manufacturing processes. Nanoinformatics also fosters efficient scientific discovery and learning through data mining and machine learning techniques.

Organizers

Nathan Baker, Pacific Northwest National Laboratory
Anne Chaka, National Institute of Standards & Technology
Yoram Cohen, University of California, Los Angeles
Vicki Colvin, Rice University
Martin Fritts, Nanotechnology Characterization Laboratory
Charles Geraci, National Institute for Occupational Safety and Health
Mark Hoover, National Institute for Occupational Safety and Health
Sharon Ku, National Institutes of Health
Kristen Kulinowski, Rice University
Phil Lippell
James Luo, National Institutes of Health
Michael McLennan, Purdue University
Jeff Morse, National Nanomanufacturing Network
Michele Ostraat, RTI International
Krishna Rajan, CoSMIC -- Iowa State University
Rebecca Reznik-Zellen, National Nanomanufacturing Network
Peter Schad, RTI International
Mark Tuominen, National Nanomanufacturing Network

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Supporting organizations include

Combinatorial Sciences and Materials Informatics Collaboratory
ICON GoodNanoGuide
nanoHUB.org
Nanoparticle Information Library
National Institute of Standards and Technology
National Nanomanufacturing Network
Nanotechnology Characterization Laboratory
Oregon Nanosciences and Microtechnologies Institute
The Safer Nanomaterials and Nanomanufacturing Initiative

Nanoinformatics 2010
Program

Wednesday, November 3
Nanoinformatics Landscape

Goal: To achieve a broad understanding of nanoinformatics activities both through demonstrations of existing nanoinformatics projects and through presentations of informatics activities from the nanotechnology research & development domain as well as exemplar disciplines.

8:00 – 5:15	Registration and Exhibits	
8:00 – 8:30	Breakfast	
8:30 – 8:45	**Welcome** *Travis Earles (Office of Science & Technology Policy)* **Purpose of Workshop** *Mark Tuominen (National Nanomanufacturing Network)*	**Ballroom**
8:45 – 10:05	**Project Demonstrations** *Introduction: Mark Tuominen (National Nanomanufacturing Network)*	**Ballroom**
8:45 – 9:05	**caNanoLab** *Sharon Gaheen (SAIC)*	
9:05 – 9:25	**nanoTAB** *Stacey Harper (Oregon State University)*	
9:25 – 9:45	**Development of a Multi-Criteria Decision Analysis Tool to Support Selection of Nanomaterial Studies** *Gretchen Bruce (Intertox, Inc.)*	
9:45 – 10:05	**Web Interfaced Nanotechnology ESOH Guidance System (WINGS)—An Overview** *Aaron Small (Luna Innovations Incorporated)*	
10:05 – 10:30	Break	
10:30 – 12:00	**Opening Keynotes** *Introduction: Jeff Morse (National Nanomanufacturing Network)*	**Ballroom**
10:30 – 11:15	**nanoHUB.org and the Delivery of Value to Authors and Users** *George Adams (Network for Computational Nanotechnology)*	
11:15 – 12:00	**Nanotoxicology as a Predictive Science That Can Be Explored by High Content Screening and the Use of Computer-assisted Hazard Ranking** *Andre Nel (University of California, Los Angeles)*	
12:00 – 1:00	Lunch	**The National Diner**
1:00 – 2:15	**Theme 1 Presentations: Data Collection and Curation** *Co-Chairs: Stacey Harper, Yoram Cohen, Peter Schad*	**Ballroom**
1:05 – 1:25	**Collaboration and Data Management** *Yoram Cohen (University of California, Los Angeles)*	
1:25 – 1:50	**Nanoparticle Ontology for Cancer Nanomedicine Research** *Nathan Baker (Pacific Northwest National Laboratory)*	
1:50 – 2:15	**The Collaboratory for Structural Nanobiology: Nanoparticle Structural Analysis as a Rosetta Stone** *Raul Cachau (SAIC-Frederick NCL)*	
2:15 – 2:30	Break	

2:30 – 3:45	**Theme 2 Presentations: Tools for Innovation, Analysis, and Simulation** *Co-Chairs: Anne Chaka, Mark Tuominen, Michael McLennan*	**Ballroom**
2:35 – 2:55	**Nanoparticles Toxicity: Knowledge Extraction from High-Throughput Screening Data** *Rong Liu (University of California, Los Angeles)*	
2:55 – 3:20	**Cloud Computing for Science** *Kate Keahey (Argonne National Laboratory)*	
3:20 – 3:45	**Scientific Workflow Tools** *Daniel Crawl (San Diego Supercomputer Center)*	
3:45 – 4:00	Break	
4:00 – 5:15	**Theme 3 Presentations: Data Accessibility and Information Sharing** *Co-Chairs: Michele Ostraat, Mark Hoover, Rebecca Reznik-Zellen*	**Ballroom**
4:05 – 4:25	**Considerations in the Application of Nanoinformatics to Occupational Safety and Health.** *Paul Schulte (NIOSH)*	
4:25 – 4:50	**PhenX Measures for Data Sharing, Cross-study Analysis and Data Interoperability** *Carol Hamilton (RTI International)*	
4:50 – 5:15	**The Implications of Open Notebook Science and Other New Forms of Scientific Communication for Nanoinformatics** *Jean-Claude Bradley (Drexel University)*	
6:00 – 7:00	**Poster Session and Reception**	**The National Diner**
7:00 – 8:00	**Keynote Banquet** *Introduction: Mark Hoover (NIOSH)*	**Ballroom**
7:30 – 7:40	**Remarks from the NanoBusiness Alliance** *Vincent Caprio (NanoBusiness Alliance)*	
7:40 – 8:00	**Remarks on the State of Nanotechnology** *Mihail C. Roco (National Science Foundation)*	

Thursday, November 4
Nanoinformatics Roadmapping

Goal: To stimulate discussion and launch the roadmapping activities that are the primary objective of the workshop, wherein themed groups will focus on a single set of informatics issues in depth and craft specific recommendations to address them.

8:00 – 5:15	Registration and Exhibits	
8:00 – 8:30	Breakfast	
8:30 – 10:00	**Roadmapping Set Up: Additional Perspectives** *Introduction: Vicki Colvin (Rice University)*	**Ballroom**
8:35 – 9:00	**EPA Perspectives on Nanoinformatics for Prioritization and Toxicity Testing** *Sumit Gangwal (National Center for Computational Toxicology)*	
9:00 – 9:25	**Nanoinformatics in Europe: The ACTION Grid White Paper** *Victor Maojo (Universidad Politecnica de Madrid)*	
9:25 – 9:50	**Getting to 'The 5 stars of Linked Open Data' for Nanoinformatics** *Mills Davis (Project10x)*	
10:00 – 10:30	Break	
10:30 – 12:00	**Roadmapping Set Up: Project Vignettes**	**Ballroom**

	Introduction: Phil Lippell	
10:35 – 11:35	**nanoHUB.org** *Michael McLennan (Purdue University)* **CoSMIC** *Krishna Rajan (Iowa State University)* **NIST** *Anne Chaka (NIST)* **ICON GoodNanoGuide** *Vicki Colvin (Rice University)* **Nanoparticle Information Library** *Mark Hoover (NIOSH)* **NIOSH Field Teams** *Chuck Geraci (NIOSH)* **NNN/InterNano** *Jeff Morse (National Nanomanufacturing Network)* **caNano Working Group** *Nathan Baker(Pacific Northwest National Laboratory)* **NCL Metadata Projects** *Marty Fritts (Nanotechnology Characterization Laboratory)* **NBI Knowledgebase** *Stacey Harper (Oregon State University)* **Materials Registry** *Michele Ostraat (RTI International)*	
11:35 – 12:00	**Panel Discussion** *Phil Lippell, moderator*	
12:00 – 1:00	Lunch	**The National Diner**
1:00 – 2:15	**Themed Breakouts** *Theme1: Data Collection and Curation* *Theme 2: Tools for Innovation, Analysis, and Simulation* *Theme 3: Data Accessibility and Information Sharing*	 **Ballroom I & II** **Ballroom III & IV** **Eisenhower Room**
Theme 2 additional presentations	**Nanoinformatics from the Biomedical Informatics Perspective** *G.H. López-Campos (Institute of Health "Carlos III")* **Developing a Virtual Vault for Pseudopotentials: A NNIN/C Initiative** *Derek Stewart (Cornell University)* **Using Open-Source Scripting Languages for Rapid-development of Informatics Capabilities** *Craig Versek (University of Massachusetts Amherst)*	
2:15 – 2:30	Break	
2:30 – 3:45	**Themed Breakouts** *Theme 1: Data Collection and Curation* *Theme 2: Tools for Innovation, Analysis, and Simulation* *Theme 3: Data Accessibility and Information Sharing*	 **Ballroom I & II** **Ballroom III & IV** **Eisenhower Room**
3:45 – 4:00	Break	
4:00 – 5:15	**Themed Breakouts** *Theme 1: Data Collection and Curation* *Theme 2: Tools for Innovation, Analysis, and Simulation* *Theme 3: Data Accessibility and Information Sharing*	 **Ballroom I & II** **Ballroom III & IV** **Eisenhower Room**
5:15 – 6:00	Break	

6:00 – 7:00 7:00 – 8:00	**Reception** **Networking Dinner**	**The National Diner** **Ballroom**

Friday, November 5
Nanoinformatics Roadmapping

Goal: To wrap up the roadmapping activities through report-ins and general discussion and to coordinate the pilot projects which will move activities forward to 2011.

8:00 – 5:15 8:00 – 8:30	Registration and Exhibits Breakfast	
8:30 – 10:00	**Report In and General Discussion** *Introduction: Krishna Rajan (Iowa State University)*	**Ballroom**
8:35 – 10:00	*Anne Chaka (National Institute of Standards and Technology)*	
10:00 – 10:30	Break	
10:30 – 12:00	**Pilot Planning for Nanoinformatics 2011** *Introduction: James Luo (National Institutes of Health)*	**Ballroom**
10:30 – 12:00	*Marty Fritts (Nanotechnology Characterization Laboratory)*	
12:00 – 1:00	**Closing Keynote Lunch** *Introduction: Mark Tuominen (National Nanomanufacturing Network)*	**Ballroom**
12:30 – 1:00	*Sylvia Spengler (National Science Foundation)*	

Nanoinformatics 2010
Abstracts

Project Demonstrations

caNanoLab

Sharon Gaheen
SAIC

The application of nanotechnology in cancer promises advancements in early detection, targeted therapeutics, and cancer prevention and control. The use of nanotechnology in biomedicine involves the engineering of nanomaterials to act as therapeutic carriers, targeting agents, and diagnostic imaging devices. To assist in expediting and validating the use of nanomaterials in biomedicine, the NCI Center for Biomedical Informatics and Information Technology (CBIIT), in collaboration with the NCI Nanotechnology Characterization Laboratory (NCL) and other Cancer Centers of Nanotechnology Excellence (CCNEs), has developed a data sharing portal called caNanoLab (http://cananolab.nci.nih.gov/caNanoLab/). caNanoLab provides access to experimental and literature-curated data from the NCL and other CCNEs and facilitates data sharing via the use of caBIG(r) technologies enabling semantic interoperability.

caNanoLab provides a model for representing the composition of nanomaterial types (dendrimer, carbon nanotube) and associated functionalizing entities (e.g. small molecules, antibodies). caNanoLab supports the annotation of nanomaterials with characterizations resulting from physico-chemical (size, molecular weight) and *in vitro* (cytotoxicity, immunotoxicity) assays and the sharing of these characterizations and associated protocols in a secure fashion. The caNanoLab project is expanding to include support for *in vivo* characterizations (pharmacokinetics, toxicology) of nanomaterials. To represent nanomaterials and associated characterizations, caNanoLab leverages concepts from the NCI's Enterprise Vocabulary Services (EVS) and the Nanomaterial Ontology (NPO) designed by Washington University. The caNanoLab project is collaborating with members of the biomedical nanotechnology community through the caBIG(r) Nano WG in the development of nano-TAB, a standard supporting data import/export between disparate nanotechnology systems.

Nano-TAB

Stacey Harper
Oregon State University

The field of nanomedicine faces many challenges in the development of standards to support meaningful data submission and information exchange. Numerous physico-chemical, *in vitro*, and *in vivo* assays must be addressed, with measurements currently dependent on non-standardized protocols and diverse technology types. Representing Structure-Activity-Relationships (SARs) in nanomedicine, in particular, is critical to understanding the effects of nanomaterial structure on biological activity. Unfortunately, information describing the nanomaterial including functionalizing entities and 3D structure is often represented in an undisciplined fashion. This lack of standardization has been a significant deterrent to meaningful data sharing across the nanotechnology community; few publications contain sufficient information to enable adequate interpretation of results and successful achievement of experimental reproducibility.

The nano-TAB effort aims to address data sharing challenges in nanotechnology by providing a standard means for identifying nanomaterials and characterizations in a tab-delimited format. nano-TAB is based on existing standards developed by the European Bioinformatics Institute (EBI) and the Investigation/Study/Assay (ISA-TAB) file format, which represents a variety of assays and technology types. The nano-TAB specification leverages ISA-TAB files describing investigations, study-samples, and assays and provides extensions to support nanomaterial structural information and assay measurements from the Washington University NanoParticle Ontology (NPO). The nano-TAB standard specification will enable the submission and exchange of nanomaterials to/from nanotechnology resources like the NCI's caNanoLab nanotechnology portal and the Oregon State Nanomaterial-Biological Interactions (NBI) knowledgebase; empower organizations to adopt standards for representing data in nanotechnology publications; and provide researchers with guidelines for representing nanomaterials and characterizations to achieve cross-material comparison.

The nano-TAB effort is a collaboration between a variety of organizations including the NCI, Washington University, Oregon State, ONAMI, NIOSH, Stanford University, and ISA-TAB. nano-TAB is registered as an ASTM Work Item, which facilitates a broad community outreach and input to the development of nano-TAB and other standards needed to support nanomedicine.

Development of a Multi-Criteria Decision Analysis Tool to Support Selection of Nanomaterial Studies

Gretchen Bruce
Intertox, Inc.

The database of information on nanomaterial toxicity studies is expanding rapidly and will continue, complicating the ability to identify and evaluate the quality of studies in the face of disparate data and to quickly identify those that will be most useful for furthering research. To assist researchers in identifying the "best" study or subset of studies based on a range of criteria, we are developing a multi-criteria decision analysis (MCDA)-based tool that will be incorporated into the collaborative Nanomaterial-Biological Interactions (NBI) knowledgebase currently being developed with researchers at Oregon State University (OSU). The tool will integrate with existing data repositories to identify studies that best meet criteria identified as important to stakeholders (researchers, policy makers, etc.), using a consistent, reproducible, and traceable method. Steps at the nascent stage of tool development include defining and characterizing the target user population and their priorities and objectives; characterizing information sources; establishing criteria that will be used to describe studies, which may include physical and chemical properties of the material, exposure and study characteristics, biological response measures, and indicators of study quality and reliability; and classifying studies according to these criteria. At each step in the process, we will obtain expert input from stakeholders. The tool, when complete, will prioritize information based on the extent to which it meets the criteria judged by the user to be most relevant and important.

Web Interfaced Nanotechnology ESOH Guidance System (WINGS)--An Overview

Aaron Small
Luna Innovations Incorporated

In order to streamline access to strategies and tools for quantifying and managing emerging environment, safety, and occupational health (ESOH) risks related to nanomaterials within the United States Air Force, Luna Innovations Incorporated has developed a web portal capable of providing up-to-date ESOH information in the rapidly growing field of nanomaterials. This site is known as the Web-

Interfaced Nanotechnology Environment, Safety, and Occupational Health Guidance System or WINGS. Luna Innovations Incorporated will provide a brief walk through of the four major guidance modules of the WINGS site: the Safety and Health Manager; the ESOH Profiles; the Resources section; and the Tool Kit. The site provides comprehensive guidance modules related to regulations and industry best practices. Additional tools and modules will allow the user to assess risk and implement necessary control methods prior to bringing the material on site, thus allowing for educated decision making with respect to nanomaterial handling, storage, and disposal considerations in advance.

Opening Keynote Presentations

nanoHUB.org and the Delivery of Value to Authors and Users

George Bunch Adams
Network for Computational Nanotechnology

nanoHUB.org is a model science gateway that dramatically lowers the barriers to publishing computer programs, seminars, and other educational materials. At the same time it increases the value of sharing such resources by providing to authors data about the impact of their works. Users find value in reduced costs of access and use. How can we best include data in this successful virtual organization?

Nanotoxicology as a Predictive Science That Can Be Explored by High Content Screening and the Use of Computer-assisted Hazard Ranking

Andre Nel
Division of NanoMedicine, California NanoSystems Institute and
Center for the Environmental Impact of Nanotechnology, University of California, Los Angeles

I will discuss the use of high throughput screening for *in vitro* toxicological assessment and hazard ranking that can be used for planning and following *in vivo* outcomes. I will demonstrate the use of engineered nanomaterial libraries and the use of an oxidative stress paradigm to establish a multi-parametric, rapid throughput screening procedure that can be used to screen for potentially hazardous material properties resulting in oxygen radical generation and cytotoxicity. I will describe the use of heat maps and self organizing maps in data processing and for making comparisons of mechanistic *in vitro* responses to *in vivo* response outcomes in zebra fish and mice. I will also demonstrate how this integrated predictive toxicological paradigm can be used to speed up knowledge generation about nanomaterial hazard, including the redesign of potentially hazardous material properties to render the materials safe.

Theme 1 Presentations: Data Collection and Curation

Collaboration and Data Management

Taimur Hassan, Haven Liu, Rong Liu, Robert Rallo, and Yoram Cohen
Center for Environmental Implications of Nanotechnology, California NanoSystems Institute,
and Department of Chemical and Biomolecular Engineering Department, University of California, Los Angeles

Assessment of the potential environmental impact of nanoparticles requires fundamental physical and chemical characterization of nanoparticles in order to be able to elucidate their transport in various environmental media and across environmental phase boundaries. There is also a growing concern regarding the potential adverse impact of nanoparticles on human health and other ecological receptors. Accordingly, in order to develop appropriate strategies for the safe design and use of nanoparticles, it is essential to develop adequate databases of nanomaterials toxicity and physicochemical properties. In this regard, a crucial element is the development of a collaborative framework that will enable rapid compilation and sharing of experimental data. At the UCLA/NSF Center for Environmental Implications of Nanotechnology (CEIN), the above challenge has been addressed through the development of a computerized collaboration and data management infrastructure utilizing the Microsoft SharePoint architecture. In the CEIN Data Management (CDM) approach Web Parts (custom web-based applications) have been developed (using Microsoft Visual Studio) to facilitate: (a) the maintenance of large volumes of data files and corresponding metadata; and (b) applets for automatic data extraction from uploaded researcher files. CDM features include, but are not limited to, file versioning, access security, advanced searches, online collaboration, as well as group support features such as forums, email notifications, surveys, wikis, and workflow management tools (e.g., for reviewed and authorized uploading of data files that adhere to established CEIN standards and protocols). The CDM server also enables teams to publish their own sub-webs with built-in collaboration tools for small and large teams. Various levels of secured access are provided for internal and external data sharing. Presently, CDM data content types include nanoparticle characterization, instruments and methods and toxicity data. Data files from the centralized CEIN data repository are interlinked (e.g., links among related documents, links among publications and data files as well as to characteristics of associated nanoparticle). The overall structure of the CDM approach will be described with a focus on usability of the system and user-experience with a system and its role in advancing efforts to develop decision tools for the safe design and use of nanomaterials.

Nanoparticle Ontology for Cancer Nanomedicine Research

Dennis G. Thomas, Rohit V. Pappu, and Nathan A. Baker
Pacific Northwest National Laboratory and Department of Biomedical Engineering, Washington University in St. Louis

Cancer nanomedicine research data are so diverse and voluminous that it is difficult to share and efficiently use them without informatics tools. Ontologies provide a unifying knowledge framework for annotating the data and facilitate the semantic integration, knowledge-based searching, unambiguous interpretation, mining, and inferencing of the data using informatics methods. In this paper, we discuss the design and development of the NanoParticle Ontology (NPO), which is developed within the framework of the Basic Formal Ontology (BFO) and implemented in the Ontology Web Language (OWL) using well-defined ontology design principles. The NPO was developed to represent knowledge underlying the preparation, chemical composition, and characterization of nanomaterials involved in cancer research. Public releases of the NPO are available through BioPortal website, maintained by the National Center for Biomedical Ontology. Editorial and governance processes are being developed by the National Cancer Institute (NCI) Cancer Biomedical Informatics Grid (caBIG®) Nanomedicine Working Group for the maintenance, review, and growth of the NPO.

The Collaboratory for Structural Nanobiology: Nanoparticle Structural Analysis as a Rosetta Stone

Raul Cachau
SAIC-Frederick

After the progress made during the genomics era, bioinformatics was tasked with supporting the flow of information generated by nanobiotechnology efforts. This challenge requires adapting classical bioinformatic and computational chemistry tools to store, standardize, analyze, and visualize nanobiotechnology information. The rapid convergence of information technologies around the nanobiotechnologies has spun collaborative networks and web platforms created for sharing and discussing the knowledge generated in nanobiotechnology. Key to these efforts is the implementation of new database schemes suitable for storage and for processing and integrating physical, chemical, and biological properties of nanoparticles. The inherent properties of the nanomaterials and the lack of a low-level language similar to that available in bioinformatics (the sequence space) create new challenges for these repositories. In this presentation, I will review the Collaboratory for Structural Nanobiology, a shared space designed to prototype new ways to annotate nanomaterials, emphasizing structural annotation in an open, collaborative environment designed to gather new requirements from diverse scientific fields such as bioinformatics and computational chemistry.

Theme 2 Presentations: Tools for Innovation, Analysis, and Simulation

Nanoparticles Toxicity: Knowledge Extraction from High-throughput Screening Data

Rong Liu, Sumitra Nair, Robert Rallo, and Yoram Cohen
Center for Environmental Implications of Nanotechnology, California NanoSystems Institute,
and Department of Chemical and Biomolecular Engineering Department,
University of California, Los Angeles

High-throughput screening (HTS) is a rapidly growing approach for studies of large selections of engineered nano-materials (ENMs) using multiple assays and cell types in order to evaluate the potential environmental impact of ENMs. The different toxicological assays measure toxicity effects resulting from different biological pathways. HTS data analysis provides information that is alternate to and/or complements traditional dose-response. HTS data involves multiple cell lines, a range of exposure media, exposure times and concentrations, nanoparticles of different types (and inherently of a range of physicochemical properties), and a multiple toxicity assays. Given the multidimensionality of the data sets, the development of cause-effect relationships (e.g., quantitative-structure-activity relationships (QSARs)) is a major challenge. For example, HTS data may contain few adverse effects (i.e., "hits") among a large collection of toxicity assay data. Moreover, at present the nanoparticles library size for a given study is typically small (i.e., relative to large compound databases in drug discovery or chemical QSAR development). Therefore, HTS data must first be carefully post-processed to remove redundant information and clearly identify toxic "hits" in order to enable proper generalization capability and interpretation via data-driven toxicity models. Accordingly, in the present work, a range of tools were developed and applied for feature extraction, clustering analysis, classification-based QSARs, and identification of similarity patterns to facilitate the extraction of ENM categories of common mechanisms of action. In the present study, at the UCLA/NSF Center for Environmental Implications of Nanotechnology, the application of machine-learning methods (e.g., self-organizing maps and kernel-based methods) has been applied for assessing the toxicity behavior of metal and metal-oxide nanoparticles. Specifically, we demonstrate that the extraction of cause-effect and toxicity pathways relationships is feasible even for relatively small nanoparticle libraries.

Cloud Computing for Science

Kate Keahey
Argonne National Laboratory

Infrastructure-as-a-Service (IaaS) Cloud computing is emerging as a viable alternative to the acquisition and management of physical resources. The Nimbus project works towards enabling scientific communities to leverage cloud computing by providing (1) an IaaS toolkit allowing providers to configure clouds, (2) user-level tools for contextualization and scaling allowing users to easily take advantage of IaaS, and (3) an extensible open source implementation of both allowing users to customize the implementation to their needs.

The talk will give an overview of the challenges and potential of cloud computing projects in science as well as the way in which the Nimbus project at Argonne National Laboratory addresses them. I will also describe what attracted various scientific communities to cloud computing and give examples of how they integrated this new model into their work. Finally, I will describe how scientific projects collaborating with us inspire technological development and take advantage of various Nimbus features.

Scientific Workflow Tools
Daniel Crawl
San Diego Supercomputer Center

Although an increasing amount of cyberinfrastructure technologies have emerged in the last few years to achieve remote data access, distributed job execution, and data management, orchestrating these components with minimal overhead still remains a difficult task for scientists. Scientific workflow systems improve this situation by creating interfaces to a variety of technologies and automating the execution and monitoring of the workflows.

A scientific workflow is the process of combining data and processes into a structured set of steps that implement semi-automated computational solutions of a scientific problem. Kepler is a cross-project collaboration, with a purpose to develop a domain-independent scientific workflow system. It provides an environment in which scientists can design and execute scientific workflows by specifying the desired sequence of computational actions and the appropriate dataflow. Currently deployed workflows range from local analytical pipelines to distributed, high-performance applications that can run in cluster, grid, or cloud computing environments.

The scientific workflow approach offers a number of advantages over traditional scripting-based approaches, including simplified configuration; improved reusability, maintenance and sharing; automated provenance management to capture and browse the lineage of data products; and support for fault-tolerance.

This talk presents an overview of common scientific workflow requirements and illustrates these features using the Kepler scientific workflow system. We highlight the features of Kepler in several scientific applications, as well as describe upcoming extensions and improvements.

Theme 3 Presentations: Data Accessibility and Information Sharing

Considerations in the Application of Nanoinformatics to Occupational Safety and Health
Paul Schulte
NIOSH

This presentation will describe the information needs in occupational safety and health and issues in applying informatics techniques to hazard identification, exposure assessment, risk assessment, and risk management.

PhenX Measures for Data Sharing, Cross-study Analysis and Data Interoperability

Carol Hamilton
RTI International

The use of common measures can greatly facilitate data sharing and data interoperability. For genome wide association studies (GWAS), meta-analyses that combine or compare studies is a widely accepted approach. Combining studies can increase the population size and the statistical power of the analysis. Increased statistical power is particularly relevant to the discovery of moderate associations and complex associations, such as gene-gene and gene-environment interactions. Comparing study results from different populations is considered essential to the validation of preliminary findings. The PhenX Toolkit provides the scientific community with high priority, recommended measures for use in GWAS and other large-scale studies. The Toolkit is intended to help researchers expand studies to include (common) measures that are outside of their primary research focus. The PhenX Toolkit currently contains over 200 measures (17 research domains) and will include measures for 21 research domains by the end of 2010. The Toolkit provides users with a web-based interface for searching, browsing, and selecting PhenX measures and protocols. For each PhenX Measure, the Toolkit provides a brief description of the measure, the rationale for selecting the measure, protocol(s) for collecting the measure, and supporting documentation. Measures are associated with a research domain, and may also be included in “Collections” (such as “Top 20 Measures”) and “Conceptual Groups” (such as “Lifestage”) that comprise measures that cut across the research domains. The “Smart Query Tool” offers two options: a high-specificity search through measure and protocol names, synonyms, and keywords; and a high sensitivity full-text search. The “Data Collection Worksheet” enables Toolkit users to easily integrate PhenX measures into their studies and the Data Dictionary provides variable names, identifiers, and attributes in several formats. All PhenX measures have Cancer Biomedical Informatics Grid Common Data Elements (caBIG CDEs) and are accessible using the caBIG CDE browser. Logical Observation Identifiers Names and Codes (LOINC) codes are also being developed for PhenX measures and some have been released with “Trial” status. PhenX measures, protocols and/or variables have been mapped to studies in the database of Genotypes and Phenotypes (dbGaP), the Public Population Project in Genomics’s (P3G) Data Schema and Harmonization Platform for Epidemiological Research (DataSHaPER), and to primary phenotype variables collected by the electronic Medical Records and Genomics (eMERGE) research consortium. The goal is to enable identification of PhenX variables in electroninc medical records (EMRs), clinical data repositories and other resources, promoting data sharing and cross-study analysis. A cross-reference guide linking PhenX measures, protocols and variables to standards and other identifiers is in development. The PhenX Toolkit provides the research community with freely available, well-established measures and bioinformatics tools that promote data sharing and data interoperability.

The Implications of Open Notebook Science and Other New Forms of Scientific Communication for Nanoinformatics

Jean-Claude Bradley
Department of Chemistry, Drexel University

This presentation will first describe Open Notebook Science, the practice of making the laboratory notebook and all associated raw data available to the public in real time. Examples of current applications in organic chemistry will be detailed. A description of the precursor system—Standard Modular Integrated Research Protocols (SMIRP)—will be provided, as it was applied to nanotechnology research and dissemination. Finally, the implications for Intellectual Property protection, claims of priority, subsequent publication in peer reviewed journals and the eventual automation of the scientific process will be explored.

Poster Session and Reception

1. The Center for Environmental Implications of Nanotechnology (UC-CEIN)

A. Nel, Y. Cohen, H. Godwin, A. Keller, and R. Nisbet
Center for Environmental Implications of Nanotechnology, California NanoSystems Institute, University of California, Los Angeles

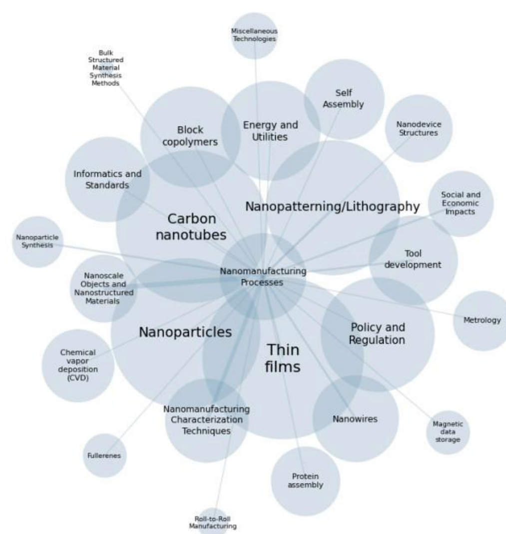
The goal of the University of California Center for Environmental Implications of Nanotechnology (UC CEIN) is to develop a paradigm for predictive toxicology and risk ranking premised on nanomaterial property-activity relationships, fate and transport analysis, exposure implications, as well as biological injury at molecular, cellular, organismal, and ecosystems levels. The integrated and multidisciplinary research effort, assisted by various modeling efforts, will help to establish functional decision tools regarding the design and safe implementation of nanotechnology. UC CEIN has successfully integrated the expertise of engineers, chemists, colloid and material scientists, ecologists, marine biologists, cell biologists, bacteriologists, toxicologists, computer scientists, and social scientists to create the scientific platform to identify possible hazards and guide the safe design of nanomaterials (NMs). Noteworthy accomplishments of the UC CEIN include (i) the development of a combinatorial library of nanomaterials (metal oxides, SWCNT, metals, clays) that includes 60 variants of nanoparticles in various stages of characterization and introduction into environmental studies; (ii) in-vitro and in-vivo studies regarding nanoparticle-induced toxicity in diverse environmental relevant systems; (iii) modeling of nanoparticle aggregation; (iv) development of an architecture for nanoparticle data management, analysis and modeling; and (v) studies on nanotechnology risk perception.

2. Interactive Taxonomy for Content Exploration and Discovery

Rebecca Reznik-Zellen, Bob Stevens
National Nanomanufacturing Network, University of Massachusetts Amherst

Interactive taxonomic functionality enables visitors to explore relationships between concepts and access content within the nanomanufacturing domain.

InterNano is an information portal and subject repository for nanomanufacturing hosted by the National Nanomanufacturing Network at the University of Massachusetts Amherst, which combines a dynamic open source content management system (Joomla!) for managing original content with the reliable EPrints repository software system for managing archived publications, educational material, and workshop presentations. Because nanomanufacturing is a small, interdisciplinary subdomain of nanotechnology, an important component of the project is a specialized taxonomy for domain definition and information discovery.



The InterNano Taxonomy is a unique, custom-built terminology to describe the nanomanufacturing enterprise—from areas of application to nanomanufacturing processes—with three levels of granularity.

The Taxonomy is fully integrated into the InterNano system, linking all tagged content both in Joomla! and in EPrints. By browsing the taxonomy either through a hierarchical list or through a tag cloud, visitors can review and access all of the tagged content within the InterNano portal and repository.

InterNano has expanded its taxonomic functionality to enable a more interactive user experience. Spring graphs display Taxonomy terms with respect to their relationship to other taxonomy terms via content tagging and reflect terms' relative usage statistics. The spring graphs are generated with open source libraries for Python: matplotlib and NetworkX. This capability allows users to explore the different concepts within the nanomanufacturing domain as well as review and access tagged content throughout the integrated InterNano system.

3. INFONANOSAFE: A Web Resource for Knowledge Integration in the Field of Nanosafety

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The Medical NanoBioInformatics Department of the Institute of Health Carlos III, as part of its contribution to the NanoSost Project [1], has designed and implemented a web portal, INFONANOSAFE, that aims to collect incoming knowledge about nanotechnology safety issues and to offer it through Internet, so becoming a reference resource in these matters for the spanish speaking community.

INFONANOSAFE website is based on Drupal CMS [2] and implements some of the cutting edge web design trends and techniques as faceted browsing, taxonomy tagging, URL rewrite, XML sitemaps and Search Engine Optimization, among others, to improve user navigation experience and search features, reducing the time to retrieve relevant data.

INFONANOSAFE categorizes the information into three axis:

- News related with the area of nanosafety and the process of characterization of nanomaterials;
- Guides designed to provide information on how to handle nanoparticles and nanomaterials, as well as their manufacturing and destruction, in order to facilitate the work of researchers and engineers;
- Catalogue of best-practices, that refers to successful experiences that can be shared in a concrete context or industrial domain.

Four lexicons, that we call facets, have been defined to be associated with documents enabling the use of advanced techniques for content retrieving and a simple and quick access to the stored documents.

a) Nanomaterial: This facet maps the family of nanoelements or nanocompounds referred by the documents. It is based on Tomalia's framework reference for classifying nanomatter [3], that could catch sight of a future nanoperiodic system and therefore predict functional properties including toxicology aspects.

b) Potential risk: Based on European directive 67/548/EEC, this facet describes potential hazards caused by nanomaterial handling (corrosive, explosive, inflammable, toxic, irritant, etc…). In order to use a more suitable classification within the field of nanoscience, it is going to be replaced by GHS—Globally Harmonized System of Classification and Labeling of Chemicals.
c) Risk management: It refers to the two most important issues that address nanosecurity—risk assessment to identify potential threats (threatened groups, measurement equipment, exposure threshold, measurement procedures, and health observation) and risk management to learn how to manage risks and to avoid its harmful consequences (engineering control, personal protection equipment, training, communication and information, organization, collective protection).
d) Economic sector: To highlight the main economic sector for which the information is relevant.

To achieve a secure development of nanotechnology it is necessary to take action in order to identify potential threats, learn to manage them, and avoid potentially harmful consequences. INFONANOSAFE will offer the user a broad spectrum of high-quality, evidence-based nanotechnology safety information accessible to the public, industry, health providers, and policy-makers.

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4. Insitu Growth of Multiwalled Carbon Nanotube on Alumina Matrix as Reinforcing Agent by Ethylene CCVD Method Using Fe as Catalyst
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We report the *in situ* growth of multiwall carbon nanotubes (MWCNT) by catalytic chemical vapor deposition (CCVD) using Fe nanoparticles as catalyst. Due to special characteristics of CNTs, such as high Young modulus, (~ T Pascal), good thermal and electrical conductivities, et cetera, these materials are known as the most suitable candidates for reinforcing metals, polymers, and ceramics composites. In this work, MWCNTs are used to reinforce Alumina matrix. We employed CCVD method to grow *in situ* MWCNT on bi powder Fe/Alumina mixed in Ball milling for two hours with different percentages. Ethylene was used as the feed gas and Argon as the carrier gas. Scanning electron microscope (SEM) and tunneling electron microscope (TEM) as well as X-ray Diffraction (XRD) and Raman spectrometer were used to characterize the synthesized nanocomposite. Results show that with an increasing percentage of Fe in the mixed powder Fe/Al, the amount of CNT in the composites increases, and the distribution of CNT in the composites improve. We also find that increasing percentage of Fe leaves more impurity particles in the composite which needs to applying various purification procedures on the synthesized composite.

5. INSCX™ Exchange: Delivering a Commercial Framework for Nanomaterials
Charles McGovern
INSCX Exchange, United Kingdom

INSCX is a patent-pending commodity exchange trading platform devoted to the trading of a wide range of nanomaterials to be launched in Europe and the United States during 2010 with global rollout to include Asia earmarked 2011. The Integrated Nano-Science and Commodity Exchange (INSCX exchange) will structure trade in accredited, compliant, and validated nanomaterials, ranging from basic raw materials such as carbons and metal oxides and advanced materials/composites to high-end, processed goods such as photonics and programmable matter.

INSCX is based in the United Kingdom and will have satellite operations in the United States and Asia. The aim of the exchange, which is supported by various companies, organizations from government in the United Kingdom, academia, the world of commodity trading and various fields of nanotechnology, is to be the focal point of the emerging world trade in nanomaterials providing tools to structure the organic growth of supply capacity in nanomaterials. The exchange process will act as a driver affording buy-side interest in the diverse suite of materials assurance on quality, transparency, and pricing in addition to permitting use of material hedging, a risk management tool offering certainty, enabling organisations to lock-in future price exposure in nanomaterials and therefore remain disposed to more confidently focus investment on research, development and other capital expenditure.

Hedging is a means to overcome price volatility where excessive volatility proves unmanageable for many parts of the supply chain. The problem posed by excessive price volatility causes immense problems in emerging materials markets especially where no effective hedging technique exists. For example, across many sectors such as the polymers industry, producers attempting to pass on rising prices to converters are meeting resistance as converters are typically under pressure from consumers to maintain previously agreed prices. This means converters are increasingly 'squeezed' in the middle, and supply chains, rather than the suppliers, are competing. Similar difficulties are already becoming manifest in the context of nanomaterials likely to compound in the absence of an effective means to plan the allocation of nanomaterials from source to end product. The structured allocation of these commodities remains the central purpose of INSCX exchange.

The opening of the exchange means that, for the first time, nanomaterials will be traded in the same way as basic commodities, adopting many of the practices and conventions long associated with formalized physical commodity trading, where the use of hedging techniques, price discovery, supplier trade financing, quality assurance, and adherence to official regulations are standard features. INSCX exchange means nanomaterials can now harness these commercial essentials with purchasers assured of quality and competitive prices, while suppliers will be provided a direct route to market, essential trade supports, and flexibilities designed to engender organic growth from within. In equal measure official regulation agencies can be confident that a formalized adherence to trade standards in the manufacture, use, application, and exchange of nanomaterials exists by way of the INSCX exchange process to support continued effort to safeguard societal interest.

6. The Knowledgebase of Nanomaterial Biological Interactions

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A risk characterization framework to classify nanomaterials based on their physical or chemical properties as well as their biological impacts is necessary to reduce the uncertainty around potential nanomaterial hazards. Structure-property relationships that can be used to predict nanomaterial impacts in lieu of empirical data can provide significant support for the nanotech industry in developing safer nanomaterials. Knowledge on the governing principles of nanomaterial-biological interactions can more effectively be utilized once computational tools are available for data integration and consensus analysis. The Nanomaterial-Biological Interactions (NBI) knowledgebase was developed to consolidate and integrate disparate data on nanomaterial effects in model systems and provide unbiased informatics approaches to identify the relative importance of characterization parameters on biological effects. The NBI serves as an open-source data repository for nanomaterial characterization, synthesis, and biological interactions, and houses a reference dataset from embryonic zebrafish evaluations on over 200 distinct nanomaterials. Various data mining and computational tools are used to organize the existing body of data in a systematic and logical way. The goal is to identify nanomaterial structure-property relationships that can be used to determine which material features can be altered to gain functionality in a predictable manner.

7. NanoGold-Bio Interaction: A Big Concern in Nanomedicine Era

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Nanotechnology is known as a set of promises to reengineer the man-made world, molecule by molecule, successfully sparking a wave of innovation in every field from mechanics to medicine. From thousands of variations of nanomaterials, gold nanoparticles (AuNPs) seem to be a promising choice as they show excellent bio-compatibility and are one of trace elements that regulate the cells coenzymes. However, as the advancement of AuNPs in the medical field increases, people come to question the safety of AuNPs. Many studies were conducted, both *in vitro* and *in vivo*, to evaluate these biological effects on human cells. Many have proved that AuNPs can induce cell damage, gene damage, but some have proven that AuNPs are not toxic and have anti-oxidative properties as well. Here, in this study, interesting data of AuNPs, compared with non-metal nanoparticles, their influence to cellular morphology, and protein interaction and level of gene expression are presented. *In vitro* alteration of cellular functions induced by nanoparticles are also presented.

8. Mosfet Analysis at Nanoscale Using Nano Simulator Version-I

Pragya Kushwaha, Sachmanik Singh Cheema ,Garima Joshi, Amit Chaudhry

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Panjab University, Chandigarh, India

9. Developing a Collaborative Environment Supporting the Application of Nanotechnology in Biomedicine

Julie Klemm[1], Piotr Grodzinski[2], Krzysztof Ptak[2], Anil Patri[3], Marty Fritts[3], Sharon Gaheen[4], Sue Pan[4], Thai Le[4], and Elizabeth Hahn-Dantona[5]

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The application of nanotechnology in cancer promises advancements in early detection, targeted therapeutics, and cancer prevention and control. The use of nanotechnology in biomedicine involves the engineering of nanomaterials to act as therapeutic carriers, targeting agents, and diagnostic imaging devices. To assist in expediting and validating the use of nanomaterials in biomedicine, the NCI Center for Biomedical Informatics and Information Technology (CBIIT), in collaboration with the NCI Nanotechnology Characterization Laboratory (NCL) and other Cancer Centers of Nanotechnology Excellence (CCNEs), has developed a data sharing portal called caNanoLab (http://cananolab.nci.nih.gov/caNanoLab/). caNanoLab provides access to experimental and literature-curated data from the NCL and other CCNEs and facilitates data sharing via the use of caBIG® technologies enabling semantic interoperability.

caNanoLab provides a model for representing the composition of nanomaterial types (dendrimer, carbon nanotube) and associated functionalizing entities (e.g. small molecules, antibodies). caNanoLab supports the annotation of nanomaterials with characterizations resulting from physico-chemical (size, molecular weight) and in vitro (cytotoxicity, immunotoxicity) assays and the sharing of these characterizations and associated protocols in a secure fashion. The caNanoLab project is expanding to include support for *in vivo* characterizations (pharmacokinetics, toxicology) of nanomaterials. To represent nanomaterials and associated characterizations, caNanoLab leverages concepts from the NCI's Enterprise Vocabulary Services (EVS) and the Nanomaterial Ontology (NPO) designed by Washington University. The caNanoLab project is collaborating with members of the biomedical nanotechnology community through the caBIG® Nano WG in the development of nano-TAB, a standard supporting data import/export between disparate nanotechnology systems.

10. nano-TAB: A Standard File Format for Data Submission and Exchange on Nanomaterials and Characterizations

Juli Klemm[1], Nathan Baker[2], Dennis Thomas[2], Stacey Harper[3], Mark D. Hoover[4], Marty Fritts[5], Raul Cachau[5], Sharon Gaheen[6]; Sue Pan[6], Grace Stafford[7], and David Paik[8]
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The field of nanomedicine faces many challenges in the development of standards to support meaningful data submission and information exchange. Numerous physico-chemical, *in vitro*, and *in vivo* assays must be addressed, with measurements currently dependent on non-standardized protocols and diverse technology types. Representing Structure-Activity-Relationships (SARs) in nanomedicine, in particular, is critical to understanding the effects of nanomaterial structure on biological activity. Unfortunately, information describing the nanomaterial including functionalizing entities and 3D structure is often represented in an undisciplined fashion. This lack of standardization has been a significant deterrent to meaningful data sharing across the nanotechnology community; few publications contain sufficient information to enable adequate interpretation of results and successful achievement of experimental reproducibility.

The nano-TAB effort aims to address data sharing challenges in nanotechnology by providing a standard means for identifying nanomaterials and characterizations in a tab-delimited format. nano-TAB is based on existing standards developed by the European Bioinformatics Institute (EBI) and the Investigation/Study/Assay (ISA-TAB) file format, which represents a variety of assays and technology types. The nano-TAB specification leverages ISA-TAB files describing investigations, study-samples, and assays and provides extensions to support nanomaterial structural information and assay measurements from the Washington University NanoParticle Ontology (NPO). The nano-TAB standard specification will enable the submission and exchange of nanomaterials to/from nanotechnology resources like the NCI's caNanoLab nanotechnology portal and the Oregon State Nanomaterial-Biological Interactions (NBI) knowledgebase; empower organizations to adopt standards for representing data in nanotechnology publications; and provide researchers with guidelines for representing nanomaterials and characterizations to achieve cross-material comparison.

The nano-TAB effort is a collaboration between a variety of organizations including the NCI, Washington University, Oregon State, ONAMI, NIOSH, Stanford University, and ISA-TAB. nano-TAB is registered as an ASTM Work Item, which facilitates a broad community outreach and input to the development of nano-TAB and other standards needed to support nanomedicine.

11. Web-Interfaced Nanotechnology Environment, Safety, and Occupational Health Guidance System–WINGS

Aaron Small, Rachel Layman, Clarissa Lynch, Morgan Williams, and Jason Shepherd
Luna Innovations Incorporated

In order to streamline access to strategies and tools for quantifying and managing emerging environment, safety, and occupational health (ESOH) risks related to nanomaterials, Luna Innovations Incorporated developed a web portal capable of providing up-to-date ESOH information in the rapidly growing field of nanomaterials. This Web-Interfaced Nanotechnology Environment, Safety, and Occupational Health Guidance System—WINGS—will be instrumental in guiding the end user through cradle-to-grave considerations for handling of nanomaterial sources. The site provides comprehensive guidance modules related to regulations and industry best practices, while also serving as a repository for related literature as well as localized medical surveillance documents. Additional tools and modules allow the user to assess risk and implement necessary control methods prior to bringing the material on site, thus allowing for educated decision making with respect to nanomaterial handling, storage, and disposal considerations in advance.

The centralization of ESOH resources through WINGS will allow Air Force personnel and OEMs to save valuable man hours by eliminating tedious searching through various sites and databases for the relevant information or regulations related to the nanomaterial of interest. Additionally, tools such as the Multi Criteria Decision Analysis (MCDA) tool will allow for rapid risk assessment through the life cycle of the nanomaterial of interest via a concise on-line questionnaire and simple scoring system. The site provides a framework that can easily be expanded to include additional data base sets, nanomaterial exposure tracking, medical surveillance tools, and information exchange forums. Additionally, the site framework is suitable for rapid modification to suit other business interests or braches of the government.

12. Nanoinformatics: Informatics for Nanomaterials Discovery and Design

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Today nanomaterials, which encompass all levels of studies and applications of materials properties revealed in unique ways under the nano-length scale, are used in numerous fields. Prompted by the highly diverse and ceaseless needs for novel functionalities of materials, the intensive efforts to extend our materials domain towards this new scale have long been continued by means of both experimental and computational approaches. At present, the nanomaterials research is guided by materials knowledge/databases accumulated over the past several decades. Along with the accelerated acquisition speed of materials data, informatics has been recognized as a powerful tool of materials research for extracting useful and comprehensive knowledge on the materials behavior from the data obtained.

In this poster presentation we discuss the application of informatics for both the design of novel functional materials, as well as for atomic-length scale characterization and analysis. In this poster presentation, we describe the application of nanoinformatics for three different fields. Applications include nanoinformatics to the analysis of nanoscale chemical imaging and characterization through atom probe tomography, design of new nanoscale biomaterials for drug delivery and finally nano-crystallography combined with informatics for the development of new inorganic scintillator materials.

13. Informatics in Relation to Nanomaterials and Worker Health
Mark D. Hoover
National Institute for Occupational Safety and Health (NIOSH)

Informatics is the science and practice of collecting, validating, sharing, visualizing, analyzing, modeling, and applying information. Modern informatics tools can be used to organize, guide, and interpret occupational safety and health research for nanotechnology specifically, and for worker protection in general. An expansion of informatics efforts is needed within the research and public health communities to ensure that risks are minimized and benefits are realized. As we attempt to move to an agreed set of minimal parameters and techniques for nanomaterial characterization, data from the use of current material characterization techniques can be organized in a manner that supports the construction of a logical taxonomy and enables the organization of materials into biologically meaningful categories. In particular, use of a categorical approach (such as grouping metal oxides or carbon-based materials according to mechanisms of toxicity versus a one-particle-at-a-time approach) will accelerate NIOSH's efforts in its key research areas of Hazard Determination (design, conduct, and interpretation of toxicology studies); Risk Assessment (dose-response evaluation of biologic effects); Exposure Assessment (metrics, methods, and the supporting research); Risk Characterization; Controls and Risk Management Methods; and Medical Screening/Surveillance and Epidemiology (including identification and tracking of nanomaterial workers who could be enrolled in exposures registries or included in epidemiological studies).

One example of an ongoing nanoinformatics initiative with which NIOSH is partnering in the National Cancer Institute's caNanoLab web-based portal (http://cananolab.nci.nih.gov/caNanoLab/), which allows researchers to share information on nanoparticles (including size, composition and other physico-chemical parameters) and information on the supporting protocols and results of in vitro and in vivo biological assays. Information from nanotechnology health and safety studies at NIOSH is available at http://www.cdc.gov/niosh/topics/nanotech/. Tools for prioritizing and controlling health risks to dangerous substances can be found at http://www.stoffenmanager.nl. The NANEX project (http://nanex-project.eu) has developed a catalogue of generic and specific (occupational, consumer, and environmental release) exposure scenarios for manufactured nanomaterials taking account of the entire lifecycle of these materials. The patient-centered, computer-based health records initiative (www.hhs.gov/healthit/ahic/healthrecords/) might support improved tracking of nanotechnology workers and improved worker health in general. Challenges for the community are to understand and improve the linkage among existing informatics initiatives; establish standards to support terminology, characterization and testing protocols, data acquisition and validation, and contents of worker health records; develop "data mining" approaches to cull the massive amounts of data from biological studies into knowledge about key parameters for occupational safety and health; and provide incentives for the community to contribute to robust platforms for nanotechnology health and safety informatics.

14. ART: Advanced REACH Tool

Chemical Safety Assessment under the European Commission's Registration, Evaluation, Authorization and Regulation of Chemicals (REACH) program can be complex and time consuming. Assessing risk requires a clear knowledge of exposure to chemicals. While Tier I models estimating exposure are available, should they be unable to show safe use, then refinement with more data or better assumptions is the only way forward. A large collaborative project is therefore initiated by TNO, bringing together leading scientist across Europe from major research organization in the field of occupational health (TNO, IOM, HSL, IRAS, BAUA and NRCWE) aiming to develop an Advanced REACH Tool (http://www.advancedreachtool.com). The ART provides a cost-effective higher tier exposure assessment approach without diminishing the protection of workers in Europe.

The ART incorporates a mechanistic model of inhalation exposure and a database of empirical exposure information from a wide variety of exposure scenarios and substances. Information from the model and the exposure database is combined using sophisticated statistical techniques to produce more refined estimates of exposure and related uncertainty. Assessors may also include their own data to update and refine estimates. The mechanistic model is calibrated using a range of data sources so that even if there are no relevant data available the ART provides useful exposure estimates.

The development of the ART started in January 2008 and received broad support from member states, industry, and ECHA and is considered as a robust and necessary way forward in exposure assessment. Several industry- and sector-specific features have been built into the ART resulting in a version 1.0 that combines the mechanistic model with a facility for statistical updates with the user’s own data. This version 1.0 was released in March 2010 and is freely available at www.advancedreachtool.com. Examples convincingly show that updating the mechanistic model estimates with available exposure data results in a substantial reduction in model uncertainty.

15. A Service-Oriented, Federated Approach for Nanoinformatics
Matt Sedlak
RJLee Group, Inc.

A federated architecture is an implementation of a Service-Oriented Architecture (SOA) centered on web services amongst an organization of systems or partners in a trust relationship called a Federation. It facilitates the secure communication of information assets amongst human and system members of a federation, where the terms of the information assurance and security are agreed upon when a system joins the Federation.

A contemporary federated solution supports distributed computing over the internet eliminating traditional point-to-point interfaces leveraging Web 2.0 (social networking) and Web 3.0 (semantic discovery) technologies with extensions for cloud and high performance computing (HPC) to support computing processing needs. Once a system defined as a “data provider” is established as part of the Federation, data is then exposed and made available to federated members. Once a system or human is defined as a “data consumer” and established as part of the Federation, data can then be accessible or discovered for consumption and sharing.

The Department of Defense (DoD) is actively implementing similar federated solutions. RJ Lee Group’s expertise within informatics and scientific solutions developed an innovative Web-Service Integration Framework Tool using open standards for the DoD as a federated baseline framework called swift. The swift toolset includes Web 2.0 Exposure services, Mashup services, Widget services, Federated Security services, and Web 3.0 Discovery services.

The Exposure services quickly enable an organization to expose data from relational databases as informational assets in the form of standard XML Web Services. The Mashup services provide system and user controlled data integration and visualization of the XML Web Services combining the data sources, data translation, and data consumption into an easy to use structure. The Mashup services are also uniquely designed for HPC of 3rd party algorithms against large data sets that are commonly found within Scientific, Engineering, and Research communities. The Widget services consume the XML Web Services providing users with a customized web application (widget) on specific functionality using Web Services for Remote Portlets (WSRP) standards. The Discovery services provide a “Google-like” natural language semantic search on exposed data sources that allow users to easily and quickly discover valuable information assets that are part of the Federation. The Federated Security services provide cross-domain application level security assurance for the swift services (exposure, discovery, mashup, widgets) by establishing a contract or trust relationship with the disparate information systems within the Federation. The security is customizable to satisfy requirements for the enterprise and is independently built on-top of an organizations existing network level security.

The Service-Oriented, federated approaches developed for the DoD can also be adopted and applied to nanoinformatics supporting the nanotechnology domain. Utilizing these approaches and technologies correctly can provide an unprecedented capability to the scientific, engineering, research ,and academic communities enabling the accessibility and sharing of nano data without geographic boundaries for the advancement of nanotechnology worldwide.

16. NANOSAFEWARE™: Compliance Management Software for Industries Supported by Emerging Nanotechnologies

Matt Hull
NanoSafe, Inc.

Much speculation remains as to whether and to what extent nanotechnology driven industries will be regulated. What is clear, however, is that as best practices and guidance strategies continue to emerge with remarkable frequency, management of key nanotechnology health and safety risks in the laboratory and workplace is becoming increasingly complex and difficult to verify. This poster presentation will describe NANOSAFEWARE™, which is an electronic compliance monitoring tool suited specifically for industries supported by emerging nanotechnologies. The program, which has been adapted from heavily regulated industries where compliance with state and federal regulatory standards is a frequent challenge, simplifies and streamlines document management, workflows, process control, workforce training, auditing, and enforcement, and keeps users updated on state-of-the-industry compliance requirements—regardless of whether such requirements are motivated by government regulations or organization specific standards of performance and safety. With representatives from both the legal and insurance communities urging organizations to minimize future liabilities by adopting proactive risk management strategies, tools like NANOSAFEWARE™ should play an increasingly important role in the organization, implementation, and verification of such strategies.

17. Pilot of the Communication and Education Message and Audience Planning Tool for the Nanoinformatics 2020 Roadmap and Plan: Illustration of Findings Related to Public Perception

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The Nanoinformatics 2010 Workshop is designed as a community-wide, public forum to survey the current nanoinformatics landscape, to stimulate collaborative activities and pilot projects, and to craft a broad-reaching Nanoinformatics 2020 Roadmap and Plan for the development and implementation of informatics in the nanotechnology domain. The draft roadmap that will be discussed at the workshop includes a table illustrating the concept of "A Communication and Education Message and Audience Planning Tool for the Nanoinformatics 2020 Roadmap and Plan". The table recognizes a diversity of stakeholders and community roles that can make informatics contributions and have informatics needs, including workers, health and safety practitioners, management, policy makers and regulators, equipment and system vendors, consumers, the legal community, researchers, educators, the media, and society in general. The table further recognizes the common and potentially unique needs of each stakeholder and partner to (1) Emphasize literacy and develop critical thinking; (2) Develop and use real-life data examples; (3) Stress conceptual understanding rather than mere application of procedures; (4) Foster continuous improvement and active discussions; (5) Use technology for developing conceptual understanding and for analyzing and sharing information (e.g., modeling and simulation, databases, etc.); and (6) Use assessments to improve and evaluate the efficacy and impact of these activities.

Success of the Nanoinformatics 2020 Roadmap and Plan will require detailed considerations of how the vision of a communication and education message and audience planning tool can be specifically and effectively refined and applied across the many disciplines and many aspects (both scientific and societal) of nanotechnology research, development, and application. In this pilot illustration an example table was prepared to stimulate discussion of possible Pilot Project ideas for application of the Communication and Education Message and Audience Planning Tool proposed in the Nanoinformatics 2020 Roadmap and Plan. Current entries represent portions of a first layer of evidence-based communication considerations for the perception of nanotechnology. Subsequent dimensions of the matrix could include parallel information related to other areas of interest such as health and safety, technical feasibility, economics, and population disparities. (The invaluable contributions of Dr. Mark D. Hoover of the National Institute for Occupational Safety and Health to this work are gratefully acknowledged.)

Roadmapping Set Up: Additional Perspectives

EPA Perspectives on Nanoinformatics for Prioritization and Toxicity Testing

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The U.S. Environmental Protection Agency's (EPA) Office of Research and Development (ORD) is investigating the environmental health and safety implications of engineered nanomaterials. Research activities as outlined in ORD's Nanomaterial Strategy (http://www.epa.gov/nanoscience/files/nanotech_research_strategy_final.pdf) address four main themes in: 1) identifying sources, fate, transport, and exposure; 2) understanding human health and ecological effects; 3) developing risk assessment approaches; and 4) preventing and mitigating risks. Under the second theme, EPA's National Center for Computational Toxicology (NCCT) is working to include evaluation of nanomaterials in its ToxCast™ chemical prioritization program. ToxCast is a battery of *in vitro*, high-throughput screening (HTS) assays that the EPA is using to develop methods to predict potential for toxicity of environmental chemicals. Design and conduct of the ToxCast pilot for screening nanomaterials requires selection of testing concentrations, characterization of materials, and analysis of resulting HTS data. Material testing concentrations are being selected by using the open-source Multiple-Path Particle Dosimetry (MPPD) model (from Applied Research Associates, Inc. (ARA)) to calculate nanomaterial mass retained in the alveolar region of the human lung based on occupational-setting aerosol levels curated from the literature. In collaboration with the Center for the Environmental Implications of NanoTechnology (CEINT) at Duke University, nanomaterial physicochemical properties are being characterized to aid in interpretation of test results. Data collection, curation, and analysis for the ToxCast nanomaterial pilot as well as for ORD-wide research on implications of nanomaterials will be facilitated using several databases developed within the NCCT. These include the Aggregated Computational Toxicology Resource (ACToR), ToxMiner, ExpoCast-DB, and the virtual tissues knowledgebase (VT-KB). Results of nanomaterial ToxCast screening and physicochemical characterization will be publicly accessible through ACToR.

This abstract may not necessarily reflect U.S. EPA policy.

Nanoinformatics in Europe: The ACTION-Grid White Paper

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ACTION-Grid [1,2] has been the first European Commission (EC)-funded initiative analyzing Nanoinformatics and its relationship with areas such as Biomedical Informatics (BMI) and Nanomedicine. This analysis was aimed towards helping develop a roadmap for future research, which has been the goal of the ACTION Grid project and the White Paper delivered to the EC.

We carried out an analysis of the state of the art and the literature—using text mining and information retrieval techniques—a survey delivered to professionals in various continents, the preparation and discussion of a large number of questions, various meetings and exchanges over the Internet, and, finally, the iterative improvement of the final draft within a Web-based collaborative space.

As a summary of this White Paper, we suggested:

- A summary of concrete actions that could be adopted by research agencies—and, in particular, the EC—to foster new developments in Nanoinformatics.
- To propose five Grand Challenges in Nanoinformatics, directly connected to BMI, which could lead to strong research results in the mid- and long- term.

In brief, these five Grand Challenges are:

1. Research on data, repositories, and standards, regarding a Nanoinformatics infrastructure for collecting, curating, annotating, organizing and archiving the available data.

2. Interoperability (semantic search, ontologies). Structuring nanomedical knowledge is essential for advancing research. Developing new ontologies at the nano level and linking them with others—e.g.,

from the OBO foundry—will facilitate future interoperability of different information systems containing nano-related data.

3. Linking nano-related data to Electronic Health Records. For instance, new standards for storing data or augmenting clinical vocabularies and terminologies—like SNOMED—or for messaging—like HL7—can incorporate nano-related terminologies and procedures, taking into account patient safety and possible secondary effects of nanoparticles.

4. Translational Nanoinformatics. A broad, integrative vision of BMI helps integrate molecular and clinical data for scientific discovery. From such a viewpoint, translational nanoinformatics requires a deeper perspective beyond current approaches to informatics, commonly linked to collecting, representing, and linking information and managing system and semantic heterogeneity. Basic scientific research at the nano level—e.g., quantum dots for imaging applications—will surely lead to new clinical applications.

5. Extension of the European Virtual Physiological Human (VPH) framework to the nano level. The VPH programme was designed for supporting R&D of patient-specific computer models and informatics tools for modeling and simulating human physiology and disease processes. In addition, there is the need to create catalogues of nanoparticles and biological targets, their interactions and potential nanotoxicity. In this context, BMI and VPH researchers have created a large number of models and simulation tools that could be reused or adapted to nanomedicine.

Finally, nanoinformatics research carried out by members of this consortium include those related to text mining approaches for a variety of topics, like extracting nanotoxicity information from the literature, linking ontologies from the nanoinformatics area with those from other areas—like the OBO Foundry—and creating repositories of various types of information that can be used for additional research, information management, and analytical efforts in nanoinformatics and nanomedicine.

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Getting to "The 5 stars of Linked Open Data" for Nanoinformatics

Mills Davis[1] and Brand Nieman[2]
1. Project10x; 2. Semanticommunity.net

Tim Berners-Lee has suggested recently implementing Open Linked Data as part of a continuum of web publishing activities associated with gold stars, like the ones you got in school, as follows: make your stuff available on the web (whatever format); make it available as structured data (e.g. excel instead of image scan of a table); non-proprietary format (e.g. csv instead of excel); use URLs to identify things, so that people can point at your stuff; and link your data to other people's data to provide context.

This presentation will illustrate and demonstrate each of these 5 stars with the Nanoinformatics 2007 and 2010 Workshop content using Wiki, business intelligence analytics and visualization, and concept-map ontology environment softwares.

Roadmapping Set Up: Project Vignettes

nanoHUB.org: An Online Resource for Research, Education, and Collaboration in the Nanotechnology Community
Michael McLennan (Purdue University)

In 2002, the NSF established the Network for Computational Nanotechnology (NCN) with a mission to connect users in research, education, design, and manufacturing by creating a national resource for theory, modeling, and simulation in nanotechnology. Users access this cyberinfrastructure from the nanoHUB.org web site. In 2009, nanoHUB.org served 274,000 visitors from 172 countries worldwide. Of these, a core audience of more than 100,000 users watched seminars, downloaded podcasts and other educational materials, and accessed more than 160 nanotechnology simulation tools. While accessing the tools, users launched a total of 369,000 simulation runs via their web browser and spent 7,286 days interacting with tools and plotting results.

nanoHUB.org supports both education and research. In 2009, 116 graduate and undergraduate classes at 97 institutions made use of nanoHUB.org in class, 50 for the first time that year. To date, 575 papers in the scholarly literature cite various resources on nanoHUB.org. In turn, these 575 papers are cited on average 6.1 times, to a total of 3,521 citations, and nanoHUB.org has an h-index of 27. Experimental data is reported alongside simulation results in 142/469 (30%) of the nano research papers that cite nanoHUB.org, indicating a clear impact on experimental research.

Simulation activity on nanoHUB.org is powered by a unique middleware that helps connect the dots between a scientific code and an end user. Code developers create a project area on nanoHUB.org, upload their code, build it, test it, and publish the final result as a tool that others can run. End users find the tool, press a button to launch an interactive session, and then interact with a graphical user interface (GUI) to set input parameters, run jobs, and visualize results. The GUI is generated automatically from an XML description of program inputs and outputs by a toolkit called Rappture, the Rapid Application Infrastructure. Rappture has an application programming interface (API) that can handle codes written in C/C++, Fortran, MATLAB, Java, Python, among other languages, and has been used by hundreds of developers to create a few hundred tools published on nanoHUB.org and other hubs.

Other activities on nanoHUB.org are also fueled by community contributions. In addition to the tools, users upload their own seminars, tutorials, homework assignments, and other resources onto the site. They rate various contributions on a scale of 1-5 stars and provide review comments. They add suggestions for improvement on various wish lists for the tools and for the site as a whole. They collaborate in private groups, editing wiki pages and sharing documents. They pose questions and provide answers in a community forum. These capabilities empower the community to work together online, publishing results and providing insights in an entirely new way.

CoSMIC: Data Driven Discovery and design for Nanomaterials
Krishna Rajan
Iowa State University

CoSMIC (Combinatorial Sciences and Materials Informatics Collaboratory- http://cosmic.mse.iastate.edu) is an international collaborative research program focused on data driven discovery in materials science. Its central research theme is to develop new computational and experimental ways of accelerated mechanistic based discovery and design of materials using informatics methods. In this presentation, we describe activities of this center that are focused specifically in the field of nanosciences. Examples of our research activities include research in how informatics can be used to elucidate nanoscale mechanisms in materials, develop a rational design strategy for new nanomaterials, and enhance the quantitative analysis of spectral and imaging data at the nanoscale. Applications of the research include discovering new nanocluster chemistries of materials, extracting pico-scale information from high resolution imaging and other characterization techniques, and integrating nanomaterials data curation with informatics. Keeping with the pervasive theme of this meeting in the fields of health and environmental issues related to nanotechnology as well as nanomanufacturing, we shall highlight CoSMIC's work in using informatics to advancing critical materials problems in these fields. CoSMIC also serves as an education portal specifically for introducing informatics concepts in the field of materials science as well as training and research workshop activities around the world.

NIST

Anne Chaka
NIST

Data Infrastructure to Address the Prediction Challenge

The Problem: Computer models and simulations can yield inconsistent and often contradictory results

- *Range of validity of models is unknown. Models developed for point solutions are not transferable.*
- *Academic researchers and software companies don't have experimental capability to validate simulation tools, and are not rewarded for establishing where methods fail.*
- *Only the industrial elite and large national programs have been able to run expensive experiments to validate models over a narrow range of applicability.*
- *Physics-based models are predictive, but are so computationally expensive that without HPC and extensive expt data they can only be run on toy problems of limited relevance.*
- *Obtaining systematic experimental data to validate simulations is not glamorous. Very difficult to fund.*

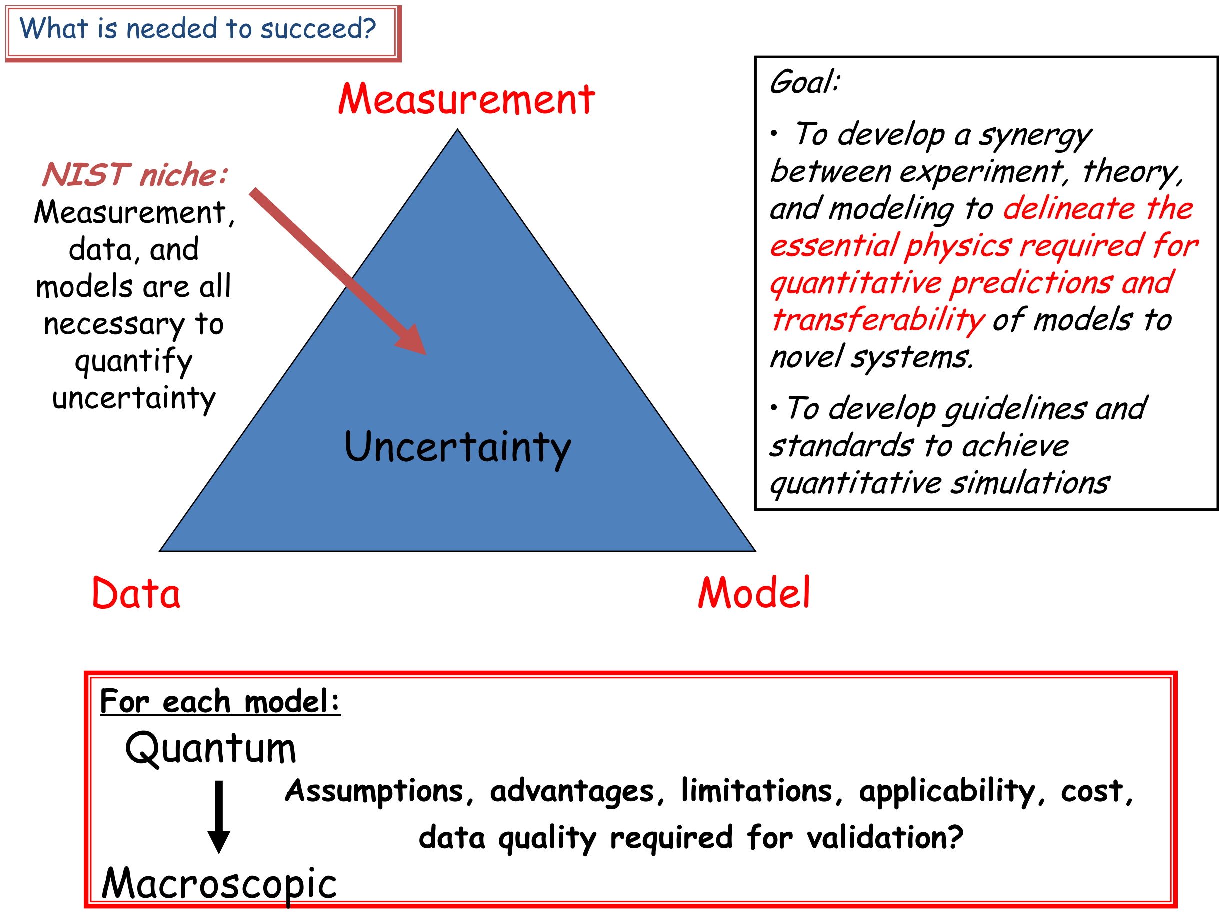
Need: Experimental data infrastructure for validation of models and simulation to drive the science forward

- *New physical measurements needed to delineate underlying science, test limits of models, and support applications of practical relevance*
- *Methodology, tolls for verification, validation, and uncertainty assessment of models and simulations*

"The prediction challenge is now the most serious limiting factor for computational science…New methods of verifying and validating complex codes are mandatory if computational science is to fulfill its promise for science and society." –**D.E. Post (LANL) and L.G. Votta (Sun Microsystems), Physics Today, January 2005.**

"…further development [of verification and validation and uncertainty quantification] will have a profound impact on the reliability and utility of simulation methods in the future." **NSF Blue Ribbon Panel, 2006.**

"The issue of model validation is crucial to regulatory approval of HPC models as an alternative to physical testing." **–Council on Competitiveness, 2004.**



Nanoparticle Information Library

Mark Hoover
NIOSH

The Nanoparticle Information Library (NIL) (http://nanoparticlelibrary.net/) was established in 2004 by the National Institute for Occupational Safety and Health (NIOSH) and its national and international partners as part of the NIOSH Nanotechnology Research Program (http://www.cdc.gov/niosh/topics/nanotech). The NIL is a searchable database of nanoparticle properties and associated health and safety information designed to help occupational health professionals, industrial users, worker groups, and researchers organize and share information on nanomaterials. The current hosting, administration, and maintenance of the NIL web resource is being conducted by Oregon State University (OSU) in conjunction with its program to characterize nanomaterials.

The information that the NIL collaborators have incorporated into the online database includes:

- Nanomaterial composition;
- Method of production;
- Particle size, surface area, and morphology (included scanning, transmission, or other electron micrographic images);
- Demonstrated or intended applications of the nanomaterials;

- Availability for research or commercial applications;
- Associated or relevant publications and links to health and safety information; and
- Points of contact for additional details or partnering.

The real-life examples of nanomaterials and their associated origins, properties, and applications in the NIL support development of a number of needed environmental health and safety tools, training aides, guidelines and standards by:

- Providing meaningful examples of the differences in nanomaterials properties that can potentially influence toxicity or the efficacy of control;
- Providing practical examples of nanomaterials and nanomaterial-associated properties to illustrate and support proposed or internationally agreed upon terminology and nomenclature, in particular, the terminology and nomenclature development initiatives of the International Standards Organization Technical Committee 229 on Nanotechnologies (http://www.iso.org);
- Supporting the development of technically defensible strategies for grouping nanomaterials into property-based categories for designing and applying controls;
- Providing catalogs of comprehensive and cost-effective measurement and assay methods for characterizing, classifying, and conducting exposure assessment for nanomaterials;
- Assembling comprehensive suites of reference materials that span the range of nanomaterials that are actually being used or are likely to be used in commerce, or can respond to specific needs for calibration of instruments or methods, or for the conduct of meaningful and intercomparable toxicology studies;
- Providing validated examples of effective control technologies for material-specific and process-specific applications; and
- Fostering insights and effective strategies to anticipate, recognize, evaluate, control, and confirm the adequacy of existing and emerging nanomaterial environmental health and safety risk management.

National Nanomanufacturing Network and InterNano

Jeff Morse
National Nanomanufacturing Network, University of Massachusetts Amherst

The National Nanomanufacturing Network (NNN) is an alliance of academic, government, and industry partners that cooperate to advance nanomanufacturing strength in the U.S. The goal of the NNN is to build a network of experts and organizations that facilitate and expedite the transition of nanotechnologies from core research and breakthroughs in the laboratory to production manufacturing. Partners and affiliates will find value added through a range of services, including training and education, industrial vision and roadmap development, thematic conferences and workshops, and a comprehensive online information resource for nanomanufacturing, InterNano.

The NNN is funded and coordinated by the NSF Center for Hierarchical Manufacturing, a Nanoscale Science and Engineering Center (NSEC) at the University of Massachusetts Amherst, and works in cooperation with the three other nanomanufacturing NSECs—the Center for High-Rate Manufacturing at Northeastern/UMass Lowell/UNH, the Center for Scalable and Integrated Nanomanufacturing at UCLA/Berkeley, and the Center for Nanoscale Chemical-Electrical-Mechanical Manufacturing Systems at UIUC—other academic research centers, as well as participants from NIST, DOD, DOE, NIH, NIOSH, and other institutions.

InterNano (http://www.internano.org), a service of the NNN, supports the information needs of the nanomanufacturing community by bringing together resources about the advances in applications, devices, metrology, and materials that will facilitate the commercial development and/or marketable application of nanotechnology. InterNano collects and provides access to information on nanomanufacturing centers, experts, and resources; nanomanufacturing news, reviews, and events; and nanomanufacturing processes, test bed reviews, and research literature, with links to best practices. It is the central, online resource through which nanomanufacturing relevant information is archived and disseminated.

InterNano is actively building a suite of informatics tools for the nanomanufacturing community, beginning with three components: a smart company and institutional directory to find and establish connections with potential collaborators; a taxonomy to explore and discover nanomanufacturing content; and a nanomanufacturing process database to share standard nanomanufacturing processes and engineered nanomaterials property information across sectors. InterNano is also currently forging partnerships that will work toward the open exchange of data through federated databases, metadata standards, and the development of advanced analytical tools for evaluating trends within the nanomanufacturing community.

InterNano represents the crossroads where issues of lab-scale scientific research intersect with the industry-scale issues of EHS, regulation, market research, and entrepreneurship. As such, the availability of consistent and reliable materials and process information, effective modeling and analysis tools, and trusted standards and protocols for information sharing with respect to intellectual property rights are all very relevant challenges that InterNano and the NNN are invested in addressing.

Oregon Nanoscience and Microtechnologies Institute and the Nanomaterial-Biological Interactions Knowledgebase

Stacey Harper
Oregon State University

ONAMI, the ***Oregon Nanoscience and Microtechnologies Institute***, is the first Oregon Signature Research Center. A cooperative venture among government and world-class nanoscience and microtechnology R&D institutions and industry in the Northwest, ONAMI was created to cultivate research and commercialization to advance the leading economic sector in Oregon and expand the benefits of technology innovation to traditional and natural resource industries. Environmental health and safety are key considerations across all ONAMI research activities. ONAMI firmly supports the idea that nanotechnology, pursued correctly, can improve our quality of life without safety or environmental risks.

A major research thrust of ONAMI is the ***Safer Nanomaterials and Nanomanufacturing Initiative*** (SNNI). The goals of the SNNI are to develop new nanomaterials and nanomanufacturing approaches that offer a high level of performance, yet pose minimal harm to human health or the environment. Research under the Initiative merges the principles of green chemistry and nanoscience to produce safer nanomaterials and more efficient nanomanufacturing processes. SNNI is confronting concerns about the biological impact of nanoparticles and has supported the development of a ***Nanomaterial-Biological Interactions (NBI) Knowledgebase (http://nbi.oregonstate.edu).*** The NBI knowledgebase serves as a repository for annotated data on nanomaterial characterization (e.g. purity, electronic and photonic properties, size, shape, charge, composition, functionalization, agglomeration state, etc.), synthesis methods, and nanomaterial-biological interactions (i.e. beneficial, benign, or deleterious) defined at multiple levels of biological organization (e.g. molecular, cellular, or organismal); thus providing the framework to conduct species, route, dose and scenario extrapolations and identify key data required to predict the biological interactions of nanomaterials. We are currently cataloging nanomaterials with as much detail (characterization and synthesis methods) as possible in order to establish useful metrics and mathematically define the relationships between physicochemical properties/synthesis methods of diverse nanomaterials and their biological interactions.

NBI was designed to enhance dissemination of critical data and information on nanomaterial hazards to industry, academia, regulatory agencies, and the general public. This expert system is being further developed to predict the toxic potential of unsynthesized nanomaterials, provide the computational and analytic tools to suggest material design or redesign that may minimize hazard, and propose experimental platforms/methods most predictive of nanomaterial-biological interactions. Features of the NBI knowledgebase will allow for unbiased interpretations of nanoparticle-biological interactions, discovery of unique structural characteristics that govern nanomaterial-biology interactions, and determination of critical data required to predict effects from nanomaterial exposure.

Materials Registry
Michele Ostraat (RTI)

The Nanomaterials Registry is an ambitious and much needed resource for the nanotechnology community. This project is funded by the National Institute of Biomedical Imaging and Bioengineering (NIBIB), the National Institute of Environmental Health Sciences (NIEHS), and the National Cancer Institute (NCI) as a contract to RTI International to develop the Nanomaterials Registry.

In this multi-year project, RTI is working to establish a web-based registry that will provide a public resource of curated information on the biological and environmental interactions of well-characterized nanomaterials. This registry, besides being an authoritative source, will provide additional information, including links to associated publications, modeling tools, computational results, and manufacturing guidance. Through this project, the team will also work to

- Create and effectively facilitate an Advisory Board of domain experts that span stakeholder groups and technology expertise;
- Develop an effective means to search, query and report on nanomaterial data and associated information by leveraging consensus-generated sets of Minimum Information About Nanomaterials (MIAN) and a logical nanomaterial ontology that spans broad biological and environmental implications;
- Design and implement a curation process to organize and evaluate information into a web-accessible database that is user-friendly and engaging to nanomaterial users and the public alike; and
- Maximize opportunities for public and professional participation and comment and to educate interested professionals and individuals on nanomaterial data relevant to biological and environmental implications through outreach and other communication activities.

As a public resource, the registry is being designed to facilitate data validation and data quality improvement of nanomaterials by the research community; enhance the development of new models, assays, standards, and manufacturing methods; and accelerate the translation of new nanomaterials for biomedical and environmental applications. This activity will also specifically address such diverse activities as regulation, product development, and environmental remediation and will allow for the integration of diverse data sources in this field.

Information exchange and data sharing is a critical component to this program, as the registry is being designed to leverage existing resources, communities, and databases already constructed and those under development. By providing an overview of the registry goals and objectives, additional opportunities for sharing can be identified early in this project.

Roadmapping Breakouts: Theme 2 additional presentations

Nanoinformatics from the Biomedical Informatics Perspective

G.H. López-Campos, V. López-Alonso, and F. Martín-Sánchez
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Along the last two decades the advances and cooperation between computer sciences, biology and medicine have allowed the development of new approaches such as genomic or personalized medicine [1]. Bioinformatics played a key role for the advance of genomic medicine supporting data management and developing new tools and methods to analyze a deluge of heterogeneous data sources. More recently, the advances in nanotechnology and their applications and uses in medicine are shaping the field of nanomedicine. Within this context, the community of users, from nanotechnology researchers to clinicians, will need a sound informatics framework, analogous to the one that is currently available from the bioinformatics discipline. From this perspective, it could be very useful to learn from the experiences accumulated in the development of genomic medicine through the collaboration forged between bioinformatics, medical informatics, molecular biology, and medicine to overcome some of the barriers that appeared along that process.

In nanomedicine the collaboration between the different players should start from the very beginning, identifying those informatics tools and methods that will be key for the advance of the discipline. The guidelines for the characterization of nanomaterials, the development of standards for data and experiment annotation, and the development of ontologies for these purposes are issues that should be addressed as early as possible. Therefore, the experience accumulated by the bioinformatics community in the development and adoption of standards such as MIAME and MAGE [2] could represent an example of the type of work to be done. Another challenge consists in the identification of those major bioinformatics resources that although having been designed for their use in genomic medicine, could be adapted for their use within nanoinformatics:

- Distributed genome annotation systems such as DAS or Ensembl ;
- Database integration systems such as Entrez or SRS;
- Gene finding and protein structure prediction programs;
- Systems Biology approaches and tools which could useful to model interactions and effects of nanoparticles in living cells and organisms.

Another challenge that must be considered is the need to adapt existing medical information systems to be able to deal with these new data sources arising from the nanotechnology field. For example, the new systems that work with nanotechnology-based imaging techniques should be compliant with the

DICOM standard, widely used for medical image management [3]. New clinical decision support systems should also be designed to deal with the new available nano-information.

Bioinformatics and medical informatics started their collaboration only recently responding to requirements posed by genomic medicine. We should avoid this delay in nanomedicine enabling a close collaboration between bioinformatics and nanoinformatics from now on. This perspective would be compliant with the concept of biomedical informatics, which pursues the efficient management of information at any level of biological organization (atom, molecule, cell, tissue, organ, individual, population) in order to advance in the development of new preventive, diagnostic and therapeutic solutions [4].

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Developing a Virtual Vault for Pseudopotentials: A NNIN/C Initiative

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Cornell Nanoscale Facility, Cornell University

First principle simulations using approaches like density functional theory have become an important tool in understanding the properties of materials and nanostructures. In some cases, these techniques have even demonstrated powerful predictive capabilities that have led to the discovery of new materials and physical phenomena. Given the widespread use of these approaches, it is important to develop cyberinfrastructure resources that provide trusted calculation components to the scientific community. Density functional simulations based on plane wave pseudopotential approaches provide the dominant approach for computational modeling of materials and nanostructures and several software packages are available at little or no cost. Pseudopotentials provide a computationally efficient way to describe the scattering of electrons from ions in a material. While electron scattering from atoms can be described using the full ion potential, this requires a large plane wave basis set and leads to time consuming calculations that dramatically limit the number of atoms that can be considered in a system. By designing shallower pseudopotentials that require a smaller basis set, yet still provide near identical scattering properties, plane wave pseudopotential codes can simulate much larger scale atomistic systems. However, the design of these pseudopotentials is still something of a black art and researchers spend a great deal of time validating pseudopotentials on standard systems before they can be used with confidence in a research setting. In addition, since different codes have different pseudopotential formats, the transfer of pseudopotentials between codes has been fairly limited.

To address these issues, the National Nanotechnology Infrastructure Network Computation Project (NNIN/C) has developed a Virtual Vault for Pseudopotentials. This cyberinfrastructure resource contains a centralized clearinghouse for information related to pseudopotentials (online collections, translators, generators, and references). In addition, we have developed a PHP-SQL database of pseudopotentials that can be accessed online. This database contains over 600 pseudopotential files drawn from several different plane wave codes. Users can interface this data through an online periodic table to find information related to a particular atom. Users can also search the database based on a given element and compare available pseudopotentials based on criteria such as exchange-correlation functional, pseudopotential class (i.e., ultra-soft, norm-conserving), parent electronic structure code, and more. This database provides the first centralized resource for pseudopotentials that spans multiple electronic codes. I will also discuss our current effort to provide metrics of pseudopotentials, including the plane wave cutoff required, predicted lattice constant and bulk modulus. In the near future, users will also have the ability to upload new pseudopotentials for evaluation, list published papers that used the pseudopotential, and also provide comments for proper usage.

Using Open-Source Scripting Languages for Rapid-Development of Informatics Capabilities

Craig Versek, Michael Thorn, and Mark Tuominen
Department of Physics, University of Massachusetts Amherst

Our experimental physics group specializes in the fabrication and characterization of materials and nanoscale systems with novel physical properties. We frequently use both commercial and custom test equipment setups to conduct material properties measurements, which require long-running and repetitive control of multiple instruments. Such laboratory tasks have already benefited greatly from in-house developed computer automation, improving the reliability of data acquisition and freeing up scientists for more creative tasks. However, the analysis of the characterization measurements often involves repetitive calculation and plotting of numerous data sets. Large volumes of data become increasingly difficult to handle using manual "spreadsheet" analysis techniques; instead, researchers might write custom programs to batch process the raw data into more meaningful parameters and visualizations. The combined automation of data acquisition, processing, organization, and visualization is the hallmark of informatics systems which have proven successful in the fields such as biology and high energy physics. The current informatics paradigm relies on massive collaborative efforts developing highly specific hardware and software infrastructure to collect vast amounts of mostly homogeneous data. However, the bewildering heterogeneity and incompatibility of the software interfaces and data formats for the instrumentation used in material science and nanotechnology research present a significant challenge to the developers of experimental informatics systems in this field.

Instead, we propose that small research groups can leverage the power of open source software and high-level scripting languages (e.g., Python, TCL, Perl, or Ruby) to knit together existing tools, each of which excel at various parts of the complete informatics package. "Open source" refers to software (and some hardware) products with licenses that protect the end users' rights to access and modify the original source materials, like human readable program code. Moreover, the open source paradigm encourages public collaborative development and sharing of knowledge, with the goals of producing interoperable and robust applications, typically free of charge. The above mentioned scripting languages are themselves open source software environments that are specifically designed to coordinate, or "script," other components as well as perform other general purpose programming tasks, while promoting gains in developer productivity.

In this talk, we present examples from actual applications developed in our lab. We describe our usage of agile software development methodologies and our selection of Python as one of the most promising programming languages for laboratory informatics. The emphasis will be on the rapid-development of custom software tools for scientific work-flow management, computer-assisted data processing, reduction, and enhanced visualization.

Nanoinformatics 2010
Speaker Biographies

George B. Adams III received the BSEE degree from Virginia Polytechnic Institute and State University in 1978 and the MSEE degree in 1980 and PhD degree in 1984 from Purdue University. In 1983 he joined the founding team of the Research Institute for Advanced Computer Science at the NASA Ames Research Center, where his work focused on high-performance computing for scientific applications. In 1987 he joined the faculty of the School of Electrical Engineering, Purdue University. He has written over 50 papers and book chapters, held one US patent, and received national awards for his distance education classes. Beginning in 2000, he was a member of the planning team for the Birck Nanotechnology Center at Purdue University and became the its Research Development Manager in 2004. In September 2007 he became Deputy Director of the Network for Computational Nanotechnology, the home of nanoHUB.org.

Nathan A. Baker, Ph.D., received his B.S. degree in Chemistry from the University of Iowa in 1997. In 2001, he received his Ph.D. in Physical Chemistry at the University of California San Diego under the joint guidance of Profs. J. Andrew McCammon (Chemistry) and Michael Holst (Mathematics). After a brief period of postdoctoral work in the McCammon lab, he joined the Department of Biochemistry and Molecular Biophysics at Washington University in St. Louis in 2002 and was promoted to Associate Professor with tenure in 2006. In 2010, Dr. Baker moved to Pacific Northwest National Laboratory as Chief Scientist for Signature Science. He is currently Lead for the National Cancer Institute caBIG Nanotechnology Working Group, Chair for the ASTM E56.01 Subcommittee on Nanotechnology Informatics, and Editorial Board Member for the Biophysical Journal. Dr. Baker's research is in the area of computational biophysics, nanotechnology, and informatics. He is actively involved in the development of new algorithms and software for computational biology and modeling in support of these research projects, including development of the APBS and PDB2PQR biomolecular electrostatics software packages (http://www.poissonboltzmann.org/) and the NanoParticle Ontology (http://www.nano-ontology.org/). Dr. Baker is the author of over 45 peer-reviewed articles as well as several reviews and book chapters. He has been awarded the Hewlett-Packard Junior Faculty Excellence Award by the American Chemical Society, the National Cancer Institute Cancer Biomedical Informatics Grid (caBIG®) Connecting Collaborators Award, and was an Alfred P. Sloan Research Fellow.

Jean-Claude Bradley is an Associate Professor of Chemistry and E-Learning Coordinator for the College of Arts and Sciences at Drexel University. He leads the UsefulChem project, an initiative started in the summer of 2005 to make the scientific process as transparent as possible by publishing all research work in real time to a collection of public blogs, wikis and other web pages. Jean-Claude coined the term Open Notebook Science to distinguish this approach from other more restricted forms of Open Science. The main chemistry objective of the UsefulChem project is currently the synthesis and testing of novel anti-malarial agents. The cheminformatics component aims to interface as much of the research work as possible with autonomous agents to automate the scientific process in novel ways. Jean-Claude teaches undergraduate organic chemistry courses with most content freely available on public blogs, wikis, games and audio and video podcasts. Openness in research meshes well with openness in teaching. Real data from the laboratory can be used in assignments to practice concepts learned in class. Jean-Claude has a Ph.D. in organic chemistry and has published articles and obtained patents in the areas of synthetic and mechanistic chemistry, gene therapy, nanotechnology and scientific knowledge management.

Gretchen Bruce is a senior scientist with Intertox, Inc. in Seattle, WA. She received her Bachelor of Science degree in Environmental Toxicology from the University of California, Davis in 1990 and is certified as a Diplomate of the American Board of Toxicology. She has over 20 years of experience conducting human health toxicological risk assessments, with particular focus on assessing risks associated with contaminants in water, food, and the workplace, including recent emphasis on pharmaceuticals, endocrine disrupting compounds, and nanomaterials, and developing computational models to predict risk. Ms. Bruce has also completed a number of application-specific multi-critieria decision analysis (MCDA) tools to support decisions about nanomaterial use for government and private users.

Vincent Caprio (http:// www.vincentcaprio.org) is the Executive Director of the NanoBusiness Alliance (http://www.nanobusiness.org). Mr. Caprio is one of the foremost advocates for government funding of emerging technologies at both the State and Federal levels. Mr. Caprio has testified before the state legislatures of New York and Connecticut, and has participated in the NanoBusiness Alliance's Washington, DC Roundtable for the past nine years. Mr. Caprio is the founder and event director of the 9th Annual NanoBusiness Alliance Conference which will be held in Chicago, IL September 27-29, 2010. During the past four years (2006-2010), Mr. Caprio was an invited speaker and guest lecturer on Nanotechnology at over 50 conferences. In addition, Mr. Caprio has appeared on numerous Connecticut TV and radio stations, including WICC 600AM (http://www.annkarrick.com/ThisWeek), discussing the impact of Water and Nanotechnology. Mr. Caprio graduated from Villanova University in 1979 with a B.S in Accounting and completed a MBA from Northeastern in 1987. Mr. Caprio is a member of Villanova University's Financial Club and serves as an active member of Villanova's President Club. Mr. Caprio serves on the Board of Trustees for the Easton Community Center and the Easton Learning Foundation in Easton, CT. In the summer of 2008, Mr. Caprio was appointed to the Board of Directors for the Fabricators & Manufactures Association Communications, Inc. based in Rockford, IL.

Dr. Anne M. Chaka is Senior Research Scientist, Physical Measurement Laboratory at the National Institute of Standards and Technology. After 20 years in the chemical industry, Anne Chaka went to the National Institute of Standards and Technology in Gaithersburg, Maryland, in 2001 to lead the Computational Chemistry Group. In 2006 she was tasked to serve on the staff of the NIST Director in 2006 as a science program analyst. After two budget cycles in the Director's Office, she has returned to her scientific career as a senior scientist in NIST Physics Laboratory. The focus of her career both in industry and at NIST has been to determine the fundamental factors responsible for performance and properties in chemical-based systems through physics-based predictive modeling and simulation. Active areas of research focus on answering the question "How good is that calculation?" for atomistic descriptions of complex systems, including nanotechnology, biophysics, surfaces and interfaces (ceramics, minerals, metals, and composites), fluid properties, and the mechanical properties of metals. After receiving her Ph.D. in theoretical chemistry from Case Western Reserve University in 1992, she spent 10 years at The Lubrizol Corporation as head of the computational chemistry and physics program. Previously, she has been Technical Director of ICN Biomedicals, Inc., and an analytical research chemist for Ferro Corporation. Dr. Chaka has been elected to several national positions in professional scientific organizations such as the American Physical Society, American Chemical Society, American Institute of Chemical Engineers, and the European Society for Theoretical Physics. She has organized several workshops focused on current challenges in industry and nanotechnology including *Cross-Industry Issues in Nanomanufacturing Workshop* (NIST, 2008), *Predictive Modeling of Nanomaterial Properties* (NSF, 2007), and *Joint Needs of the Semiconductor-Chemical Industries in Nanotechnology Modeling*, (NIST, 2006).

Dr. Yoram Cohen received his B.A.Sc., M.A.Sc., in 1975 and 1977, respectively, both in Chemical Engineering, from the University of Toronto, and his Ph.D. from the University of Delaware in 1981. He has been on the Faculty of Chemical and Biomolecular Engineering at the University of California, Los Angeles (UCLA) since 1981. He is the founder and Director of the Water Technology Research Center and the Center for Environmental Risk Reduction, and a member of the UCLA/National Science Foundation (NSF) Center for the Environmental Implications of Nanotechnology (CEIN). Dr. Cohen is an Adjunct Professor at Ben-Gurion University and a member of the International Advisory Committee to the Stephen and Nancy Grand Water Research Institute at the Technion. He was a Visiting Professor at the Technion (1987-1988), at Universitat

Rovira i Virgili (1944) and a Distinguished Visiting Professor at Victoria University (2006). Dr. Cohen is a UCLA Luskin Scholar and a recipient of the 2008 Ann C. Rosenfield Community Partnership Prize in recognition of his environmental research. He received the 2003 Lawrence K. Cecil award in Environmental Chemical Engineering from the American Institute of Chemical Engineers (AIChE), as well as the AIChE Separations Division Outstanding Paper Award (1997 and 2009). In 2008 he received a County of Los Angeles Commendation (2008), a State of California Senate Certificate of Recognition, and a Certificate of Special Congressional Recognition (US) for contributing to legislation to protect public health and dedicated service to the Los Angeles community. Dr. Cohen has published over one hundred and fifty research papers and book chapters in water technology, separations processes, transport phenomena, polymer science, surface nano-structuring and environmental engineering. He is also the Editor of three environmental volumes. Dr. Cohen developed patented technologies in membrane synthesis, reverse osmosis desalination, surface nanostructuring and chemical sensors. He has served on numerous Government Advisory Committees, and organized over thirty scientific conferences, including the 2008 International Congress on Membranes and membrane processes (ICOM) and the 2009 West Coast Water Technology Transfer workshop. He also was appointed as the Meeting Program Chair of the 2010 AIChE Meeting.

Dr. Vicki Colvin was recruited by Rice University in 1996, to expand its nanotechnology program. Today, she serves as Professor of Chemistry and Chemical Engineering at Rice University as well as Director of its Center for Biological and Environmental Nanotechnology (CBEN). CBEN was one of the nation's first Nanoscience and Engineering Centers funded by the National Science Foundation. One of CBEN's primary areas of interest is the application of nanotechnology to the environment. Dr. Colvin has received numerous accolades for her teaching abilities, including Phi Beta Kappa's Teaching Prize for 1998-1999 and the Camille Dreyfus Teacher Scholar Award in 2002. In 2002, she was also named one of Discover Magazine's "Top 20 Scientists to Watch" and received an Alfred P. Sloan Fellowship. Dr. Colvin received her Bachelor's degree in chemistry and physics from Stanford University, and obtained her Ph.D. in chemistry from the University of California, Berkeley. She is a frequent contributor to Advanced Materials, Physical Review Letters and other peer-reviewed journals, and holds patents to four inventions.

Mills Davis is the founder and managing director of Project10X, specializing in industry research and strategic programs. Mills consults with technology manufacturers, global 2000 corporations, and government agencies on next-wave semantic technologies and solutions. Mills serves as lead for the Federal CIO council’s Semantic Interoperability Community of Practice (SICoP) research into the business value of semantic technologies. Also, he is a founding member of the AIIM interoperable enterprise content management (iECM) working group and a founding member of the National Center for Ontology Research (NCOR).

Travis Earles serves as Assistant Director for Nanotechnology in the White House Office of Science and Technology Policy. He co-chairs the National Science and Technology Council Subcommittee for Nanoscale Science, Engineering and Technology (NSET), facilitating interagency coordination through the National Nanotechnology Initiative (www.nano.gov) and reaching out to the science and technology community across academia, government, and industry to foster responsible development of nanotechnology. Formerly at the National Cancer Institute, Earles helped plan, coordinate, and implement the five-year, $144 million Alliance for Nanotechnology in Cancer (nano.cancer.gov) launched in 2005. He holds a bachelors degree in biomedical engineering from Catholic University of America as well as an MBA and MS in technology management from the University of Maryland.

Dr. Martin Fritts is a Senior Principal Scientist supporting the Nanotechnology Characterization Laboratory and SAIC-Frederick in accelerating the transition of nanotechnology to cancer and biomedical applications. He is also a computational and experimental physicist assisting in the implementation of advanced imaging and measurement instrumentation, modeling and simulation to elucidate the structure-activity relationships of nanomaterial, and informatics systems to advance knowledge sharing. Dr. Fritts also assists in developing standards as the co-chair of ASTM's E56.02 Subcommittee on Nanotechnology Characterization. Prior to joining SAIC-Frederick, he developed and prototyped nanotechnology applications for industry and government through SAIC's Nanotechnology Initiatives Division. Dr. Fritts' previous work also focused on joint experiment and computation in advanced product and process design and the use of information technology and modeling for collaboration in large research and development projects such as laser fusion with LLNL and LANL; counterterrorism with DTRA; ship design with DARPA, NAVSEA, and industry; and the design of Stars and Stripes, the winner of the 1987 America's Cup. He earned a bachelor's degree in physics at Holy Cross College and a doctorate in nuclear physics at Yale University.

Sharon Gaheen is Program Manager of Science Applications International Corporation's (SAIC's) bioinformatics initiatives supporting the National Cancer Institute Center for Biomedical Informatics and Information Technology (NCI CBIIT) and cancer Biomedical Informatics Grid (caBIG) Program. Ms. Gaheen's program portfolio includes projects supporting the development of: service-oriented architectures enabling biomedical data integration; grid computing connecting the cancer research community; large-scale data repositories supporting expression studies; genomic-based analysis tools/algorithms; data mining/warehousing techniques facilitating translational research; technologies supporting in vivo cancer imaging; informatics supporting nanotechnology and nanoparticle characterization; standards based messaging frameworks supporting clinical research; and a variety of other applications supporting pre-clinical and clinical research. Ms. Gaheen is an Assistant Vice President at SAIC and is Deputy Division Manager of SAIC's Innovative Informatics Technologies (IIT) Division. Ms. Gaheen is an experienced IT manager and has been involved in all aspects of the software development life cycle for a variety of industries including life sciences, defense, and space sciences. Ms. Gaheen has an MBA from the University of Maryland's Smith School of business and a BS in mathematics from the University of Pittsburgh. Ms. Gaheen is a member of the National Academy of Engineering (NAE) and of SAIC's Science and Technology Fellows Council (STFC).

Dr. Sumit Gangwal is a Chemical Engineer (post-doctoral fellow) in the U.S. Environmental Protection Agency's (EPA) National Center for Computational Toxicology (NCCT). Dr. Gangwal is working on the ExpoCast™ project under the direction of Dr. Elaine Cohen Hubal. The US EPA ExpoCast™ program is aimed at developing novel approaches and metrics to screen and evaluate chemicals and nanomaterials based on biologically relevant human exposures. The goal of this research initiative is to advance characterization of exposure required to translate findings in computational toxicology to information that can be directly used to support exposure and risk assessment for decision making and improved public health. An emphasis is being placed on conducting research to mine and apply scientific advances and tools in a broad range of fields to provide information that can be used to support enhanced exposure assessments. Combining information from the ToxCast™ program, a battery of rapid screens the EPA is studying to determine whether they can predict toxicity, with information from ExpoCast™ will help the Agency determine priority chemicals and nanomaterials for evaluation based on potential to harm human health. Dr. Gangwal earned a Ph.D., M.S. and B.S. in Chemical Engineering from North Carolina State University. During his graduate studies, Dr. Gangwal's research focused on the assembly and manipulation of particles (having nanometer-sized metallic coatings) in applied electric and magnetic fields.

Dr. Charles Geraci is Coordinator of the NIOSH Nanotechnology Research Center and is also Chief of the Document Development Branch. He has over 30 years of Industrial Hygiene practice experience that has included the federal government, consulting, and private industry. Dr. Geraci earned a B.S. in chemistry from the University of Cincinnati and a Ph.D. in chemistry from the Michigan State University. He is Certified by the American Board of Industrial Hygiene in both the Comprehensive Practice and the Chemical Aspects of Industrial Hygiene and is a Fellow of the American Industrial Hygiene Association. Dr. Geraci manages a number of nanotechnology projects in the Institute and is responsible for the development of workplace guidelines, including the document "Approaches to Safe Nanotechnology". He sponsors the NIOSH nanotechnology field team that is conducting visits to nanomaterial producers and users to characterize exposures, evaluate controls, and develop best practices. As Chief of Document Development, Dr. Geraci manages projects dealing with the development of recommendations to address worker health and safety in new or emerging technologies. Dr. Geraci has made numerous presentations on nanotechnology at national and international meetings and has served as co-author on several publications dealing with risk management of nanomaterils. His research interests include development of exposure monitoring methods, evaluating the effectiveness of training, developing effective methods for risk characterization and management, and assessing the hazards and risks of new technologies.

Carol M. Hamilton is the RTI Principal Investigator for the PhenX project. Dr. Hamilton has experience in molecular biology, technology development, analysis of complex genomic and clinical data sets, development of data visualization tools, and data management.

Stacey Harper, Ph.D., is a Signature Research Faculty Fellow of the Oregon Nanoscience and Microtechnologies Institute and an Assistant Professor in the Department of Environmental & Molecular Toxicology and the School of Chemical, Biological & Environmental Engineering at Oregon State University. She earned her bachelor's degree in natural sciences and mathematics from Mesa State College, CO and her master's and doctoral degrees in biological sciences from University of Nevada Las Vegas, NV. She then served two years as a post-doctoral research fellow with the Exposure and Dose Research Branch of the EPA. In her research at OSU, she employs in vivo approaches to evaluate the biological activity and toxic potential of novel nanomaterials, and has established a collaborative, multidisciplinary research program to develop a knowledgebase of Nanomaterial-Biological Interactions (NBI).

Dr. Mark D. Hoover is a senior research scientist in the Division of Respiratory Disease Studies at the CDC's National Institute for Occupational Safety and Health, in Morgantown, West Virginia. Mark is a critical area leader in the NIOSH Nanotechnology Research Center and also serves as coordinator of the NIOSH Exposure Assessment Cross-sector Research Program. NIOSH is the leading federal agency conducting research and providing guidance on the occupational safety and health implications and applications of nanotechnology. Mark earned a BS degree in mathematics and English in 1970 from Carnegie Mellon University and MS and PhD degrees in engineering in 1975 and 1980 from the University of New Mexico. He is board certified in the comprehensive practice of health physics and in the comprehensive practice of industrial hygiene. Mark has developed improved approaches, techniques, and instrumentation for aerosol characterization, generation, and control; served as chairman or contributor to the development of many national and international standards; is a past chairman of the AIHA Nanotechnology Working Group; and is author or co-author of more than 180 open literature publications. In 2010, he completed co-editing and writing a new CRC handbook on Radioactive Air Sampling Methods. Special emphasis areas for Mark's work in nanotechnology include exposure assessment and characterization of nanoparticles in the workplace, development of a prototype Nanoparticle Information Library, and promotion of opportunities to apply performance-based occupational exposure limits or control banding approaches to nanotechnology. Detailed information about the NIOSH nanotechnology health and safety research program is available at www.cdc.gov/niosh/topics/nanotech/.

Dr. Kate Keahey is a Scientist in the Distributed Systems Lab at Argonne National Laboratory and a Fellow at the Computation Institute at the University of Chicago. Kate pioneered the use of virtual machines in distributed computing which grew into Infrastrucutre-as-a-Service (IaaS) cloud computing. A vocal advocate of cloud computing for science, she led numerous projects focused on overcoming barriers to its adoption as well as proposing and exploring now interaction patterns emerging in this context. Kate created and leads the Nimbus project, an open source cloud computing platform providing Infrastructure-as-a-Service as well as higher-level services for scientific communities.

Guillermo Lopez-Campos is a member of The Bioinformatics and Public Health Area (BIOTIC), belonging to the Applied Services, Training and Research General Subdepartment of the Institute of Health Carlos III.

Professor Victor Maojo, MD, PhD is a Full Professor and Director, Biomedical Informatics Group, UPM, Madrid. He holds a M.D. degree and a Ph.D. in Computer Science. He has been a Postdoctoral Researcher at Georgia Tech (Atlanta, USA), and at the Harvard Medical School-MIT joint program in medical informatics in Boston, USA. He has been the Principal Investigator in more than 15 national projects and has been awarded two international grants from Hewlett-Packard USA and Europe. He has been an Expert for the European Commission in the IV, V, VI and VII Framework Programmes. He has participated in ten European Commission-funded projects. He has published over 150 research papers in scientific journals and international conferences, including the invited edition of special issues of peer-review journals. He is in the editorial board of various scientific journals. He has published numerous papers in top-ranked Biomedical Informatics journals (e.g., JAMIA, Journal of Biomedical Informatics, Methods of Information in Medicine, IEEE EMB, IEEE TITB, Computers in Biology and Medicine, BMC Bioinformatics or Bioinformatics) and other publications in journals like Pediatric Research, Pattern Recognition, Nature or JASIST. Prof. Maojo has given a large number of invited and Keynote speeches and chaired various international conferences and special sessions. He has been the coordinator of the EC-funded ACTION Grid project (until June 2010) in the area of Nanoinformatics, where he has published various journal papers and actively participates in research in the area (in topics like text mining, ontologies and database integration).

Michael McLennan, Ph.D., is a Senior Research Scientist in the Rosen Center for Advanced Computing at Purdue University. He is the software architect for nanoHUB.org and creator of HUBzero's Rappture toolkit. Dr. McLennan has a long history of developing CAD software at companies including Bell Labs and Cadence Design Systems. He received a Ph.D. in 1990 from Purdue for the study of quantum mechanical electron transport in mesoscopic devices, supported as an SRC Graduate Fellow. He is also well known in the open source community for creating [incr Tcl], an object-oriented extension of the popular Tcl scripting language. He is a coauthor of two books: "Effective Tcl/Tk Programming" and "Tcl/Tk Tools."

Jeff Morse, Ph.D., is the Managing Director of the National Nanomanufacturing Network, an organization sponsored by the National Science Foundation and coordinated through the Center for Hierarchical Manufacturing at the University of Massachusetts Amherst. Previously, Jeff has been a Senior Scientist in the Center for Micro and Nano Technology at Lawrence Livermore National Laboratory since 1985. He received his BS (1983) and MS (1985) Degrees in Electrical Engineering from the University of Massachusetts Amherst and a PhD (1992) in Electrical Engineering from Stanford University. His interests and expertise includes semiconductor devices and physics, advanced micro/nanofabrication processes, microelectromechanical systems (MEMS), microfluidics, catalytic microreactors, and micro-fuel cells. Jeff's work has appeared in 15 journal publications, 45 conference presentations, with an additional 30 invited lectures at academic departments, industry research centers and technical meetings. Jeff additionally holds 15 patents in several technical areas.

André Nel is a Professor of Medicine and Chief/founder of the Division of NanoMedicine at UCLA. He is the Director of the Center for the Environmental Impact of Nano technology (CEIN), which is housed in the California NanoSystems Institute (CNSI) at UCLA. Dr. Nel obtained his M.B., Ch.B. (MD) and Doctorate of Medicine (PhD equivalent) degrees from the University of Stellenbosch in Cape Town, South Africa, and subsequently did Clinical Immunology and Allergy training at UCLA. Dr Nel served a Chair of an Immunology Study Section the NIAID, is the Director of the UCLA Asthma and Immunology Disease Center, has been included in the Best Doctors of America peer-selected list for over a decade, the recipient of the John Salvaggio Memorial Award recognizing his outstanding service to the specialty and science of Allergy and Immunology, American Academy of Asthma Allergy and Immunology (AAAAI), and is member of the AAAAI Plenary Committee. Dr. Nel was recently selected as an honorary foreign member of CAS, has been included in a WTEC panel that will be responsible for preparing a national vision for Nanotechnology in the next decade. Dr. Nel's chief research interests are: (i) Nanomedicine, including the use of a mesoporous silica nanoparticle treatment platform that can be used for drug delivery, siRNA delivery and imaging; Dr. Nel is the co-director of the UCLA Nanomachine Center that is housed in the CNSI at UCLA; (ii) Nanobiology with particular interest in interfacial nanomaterial properties that can be to improve biosafety in humans and the environment; (iii) Nanotoxicology, with particular interest on the development of predictive toxicological screening paradigm, nanomaterial safety testing, high throughput screening and establishment of Nano-QSARs, inhalation toxicology and nanomaterial impact on the environment; (iv) The role of air pollutants in asthma, with particular emphasis on the role of ultrafine particle-induced oxidative stress in the generation of airway inflammation and asthma. The research is funded by personal RO1 grants from the NIEHS and NCI, the NIAID-funded Asthma and Immunology Disease Clinical Research Center, an EPA STAR award, and a $24 million NSF award for the CEIN.

Dr. Michele Ostraat, Senior Director for the Center for Aerosol and Nanomaterials Engineering at RTI International, has expertise in aerosol technology, nanoparticle applications, submicron particle processing, micro- and nanofiber filtration, portable nanoparticle detection, occupational safety and health of nanoparticles, and inhalation toxicology. She has experience in integrating emerging market needs with technology capability to define vision and strategies for organizations, prioritizing programs for market development and commercialization. Before joining RTI, Dr. Ostraat worked at DuPont's Experimental Station with primary responsibilities in the aerosol synthesis and characterization of sub-micron and nanoparticles for a variety of electronic and materials applications. While at DuPont, she was the principal investigator for the Nanoparticle Occupational Safety and Health Consortium. Prior to joining DuPont, Dr. Ostraat was a Member of Technical Staff at Bell Labs and Agere Systems where she examined the synthesis of rare-earth doped aerosol nanoparticles and investigated the behavior of chalcogenide phase change materials. She earned her Ph.D. (2001) and M.S. (1998) degrees in Chemical Engineering from the California Institute of Technology with her Ph.D. thesis entitled "Synthesis and Characterization of Aerosol Silicon Nanoparticle Nonvolatile Floating Gate Memory Devices." She holds a B.S. Chemistry degree from Trinity University. She was a Hughes Summer Student at the University of New Mexico, a SMART Program Student at Baylor College of Medicine, and has interned at Sandia National Laboratories.

Professor Krishna Rajan leads an NSF research center focused on informatics-inspired materials design, in which new material development is guided by insights from data fusion of multi-scale data sets derived from fundamental materials theory, process sequence descriptions, and property measurements. He and his group have the expertise to provide guidance into new surface coating materials and help digitally archive the materials, processes, and experimental results.

Dr. Mihail C. Roco is the founding chair of the National Science and Technology Council's subcommittee on Nanoscale Science, Engineering and Technology (NSET), and is the Senior Advisor for Nanotechnology at the National Science Foundation. He also coordinated the programs on academic liaison with industry (GOALI). Prior to joining National Science Foundation, he was Professor of Mechanical Engineering at the University of Kentucky (1981-1995), and held visiting professorships at the California Institute of Technology (1988-89), Johns Hopkins University (1993-1995), Tohoku University (1989), and Delft University of Technology (1997-98). Dr. Roco was a researcher in multiphase systems, visualization techniques, computer simulations, nanoparticles and nanosystems. He initiated the first Federal Government program with focused on nanoscale science and engineering (on Synthesis and Processing of Nanoparticles) at NSF in 1991. He formally proposed NNI in a presentation at White House/OSTP, Committee on Technology, on March 11, 1999. He is a key architect of the National Nanotechnology Initiative, and coordinated the preparation of the U.S. National Science and Technology Council reports on "Nanotechnology Research Directions" (NSTC, 1999) and "National Nanotechnology Initiative" (NSTC, 2000).

Paul A. Schulte, Ph.D., is the Director of the Education and Information Division, and Manager of the Nanotechnology Research Center, National Institute for Occupational Safety and Health, Centers for Disease

Control and Prevention. Dr. Schulte has 35 years experience in conducting research and developing guidance on occupational cancer, nanomaterials, risk communication, and genetics. He is the co-editor of the textbook entitled, "Molecular Epidemiology: Principles and Practices." He has served as guest editor of the Journal of Occupational Medicine and the American Journal of Industrial Medicine and was on the initial editorial board of Cancer Epidemiology, Biomarkers and Prevention. He currently is on the editorial board of the Scandinavian Journal of Work and Environmental Health, and the International Advisory Board of the Annals of Occupational Hygiene.

Dr. Aaron C. Small is a Senior Research Scientist at Luna Innovations Incorporated. In his five years at Luna, he has been principal investigator on over 15 programs related to flame retardant, ballistic, and nanocomposite materials, smart adhesives, appliqués, and biocidal products as well as authored/coauthored 8 technical papers and two refereed journal articles. Prior to joining Luna Innovations, he spent 5 years at Reichhold, Inc. as a senior synthesis chemist on the Global Strategic Research and Development team for the composites business designing resin systems for open and closed molding applications. While at Reichhold, he co-authored 3 patent applications, 4 technical papers, won the DIC Bronze Award for a poster presented on two novel pultrusion products he developed and commercialized, and an award for best technical paper in the pultrusion subject matter at the ACMA 2005 show and exhibition. In his time at Reichhold, he was responsible for over 15 products that generated over 25 million pounds of business in 2004 and spanned all areas of the composites business, from pultruded sea walls for the Navy to urethane hybrid acrylic back-up resins for spas. Aaron received his Ph.D. in Organic Chemistry from The University of Michigan, Ann Arbor in 2000 and his B.S. in Chemistry from Southern Methodist University, Dallas in 1995. Aaron's thesis work was focused on developing chemical tools for controlling liquid crystalline behavior. He was also in charge of the departmental DSC and TGA for the final two years of his time at the University of Michigan and has extensive experience in thermal characterization of materials.

Dr. Sylvia Spengler is program director in Division of Information and Intelligent System (IIS) within the CISE Directorate at the National Science Foundation. She also served as program officer for the Biological Databases and Informatics in BIO/DBI. Prior to joining NSF, she was a Director of Department of Energy (DOE) Human Genome Program Field Operations. She served as Co-Director of the Program in Mathematics and Molecular Biology at the University of California, Berkeley, Lawrence Berkeley National Laboratory. Her many honors include Senior Fellow of the American Cancer Society, and National Institutes of Health (NIH) Postdoctoral Fellow. As a member of DOE ELSI panels, she has been involved in evaluating the ethical, legal and social implications of human genome research. Dr. Spengler's many publications include co-authorship of the DOE's Primer of Molecular Biology.
As part of her work with the Human Genome Project Dr. Spengler has been involved in many types of public outreach including lectures given to college students, judges, and appearances on public television. Her current NSF programs include

- Information and Intelligent Systems: Advancing Human-Centered Computing, Information Integration and Informatics, and Robust Intelligence;
- CISE Pathways to Revitalized Undergraduate Computing Education (CPATH);
- Domestic Nuclear Detection Office/National Science Foundation Academic Research Initiative (ARI);
- Explosives and Related Threats: Frontiers in Prediction and Detection (EXP);

Derek Stewart is a Scientific Computational Research Associate, managing modeling and theory, at the Cornell Nanoscale Facility (CNF)at Cornell University in Ithaca, New York. The CNF is a user facility where academic, industrial, and government researchers from across the country can come to take advantage of their unique fabrication and computational capabilities. The CNF is also part of the National Nanotechnology Infrastructure Network which provides user facilities for researchers at academic institutions across the country. Mr Stewart's work involves providing a range of modeling capabilities for nanoscale research, while at the same time working to expand the capabilities through research, code developments, and collaborations. He has also organized and hosted three computational workshops looking at a variety of nanoscale simulation techniques from nanophotonics, microfluidics, first principle approaches to nanoscience and geology.

Professor Mark Tuominen is the Director of the National Nanomanufacturing Network, Co-Director of the NSF Center for Hierarchical Manufacturing and a Professor in Physics at the University of Massachusetts Amherst. Mark has a bachelor's degree in Chemical Engineering (1986) and a PhD in Condensed Matter Physics (1990), both from the University of Minnesota. His current research includes nanomanufacturing R&D, magnetism, nanoscale charge transport, and energy devices. He currently serves as a U.S. delegate to the ISO TC-229 Committee on Nanotechnologies and as leader of the ISO nanomanufacturing terminology project.

Craig Versek is a Graduate Research Fellow in the Physics Department of the University of Massachusetts Amherst.