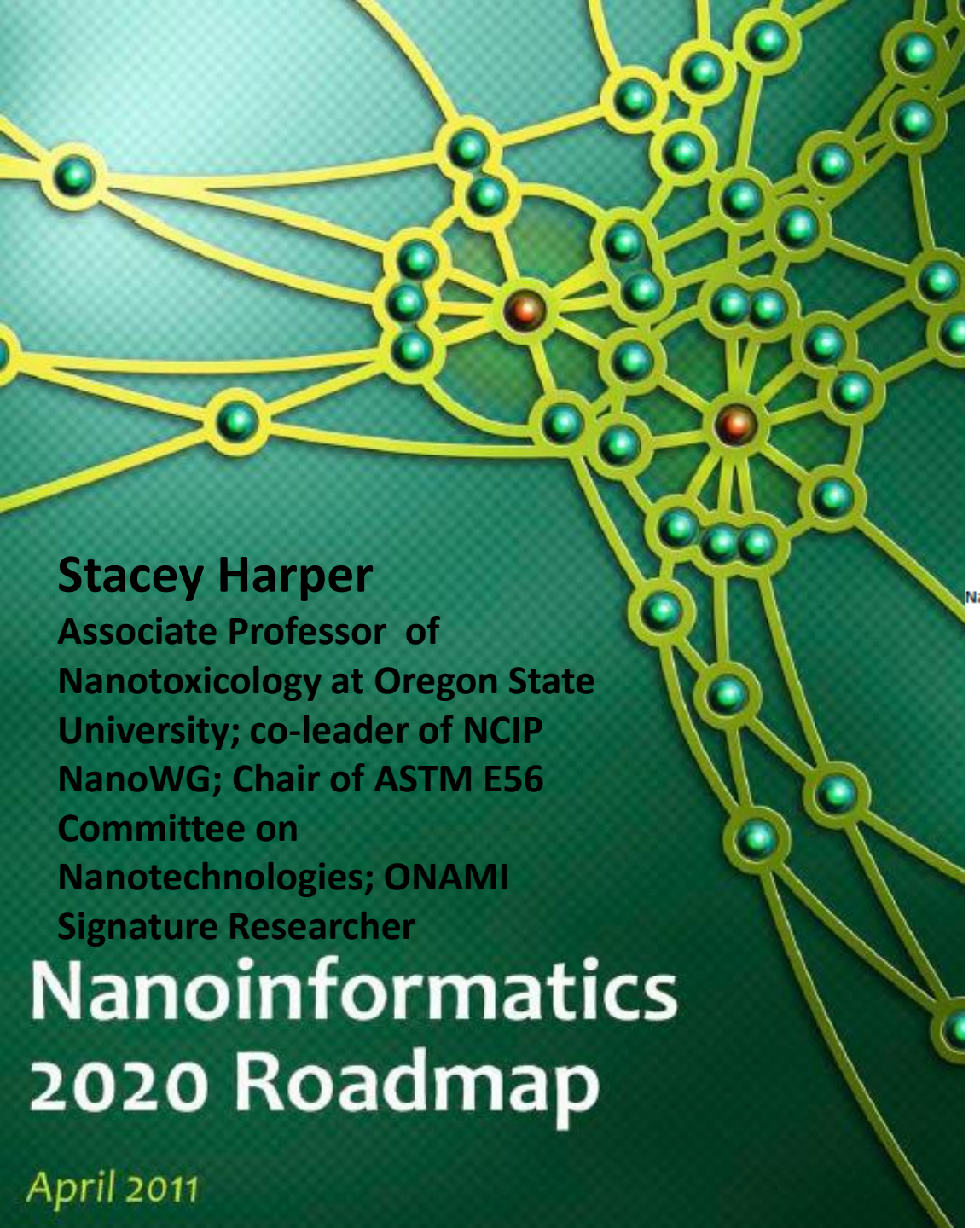

Stacey Harper

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Nanoinformatics 2020 Roadmap

April 2011

This Roadmap was prepared in concert with Nanoinformatics 2010 workshop organizers and participants, with substantial input from:

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Nanoinformatics 2010 Organizing Committee

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Goals of Nanoinformatics 2020 Roadmaping Workshop (held in 2010)

- To survey the current nanoinformatics landscape
- To stimulate collaborative activities and pilot projects
- To craft a broad-reaching *Nanoinformatics 202 Roadmap and Plan* for the development and implementation of informatics in the nanotechnology domain.

- Outcomes will:
  - Help identify stakeholders, needs, capabilities, and connections
  - Held us improve and “travel” on the roadmap to develop, understand, and apply nanotechnology in beneficial ways.

Organization of Nanoinformatics 2020 Roadmap The Skeleton

- Executive summary
- What is informatics? (definition, background and collective vision)
- The nanoinformatics commmunity (integrative view, grassroots)
  - Synopses of current projects
  - Convergence of current work products
- Cross-cutting issues
  - Vital to research and development
  - Coordination and incentives are essential for success
  - Standards for data documentation are critical
  - Successful informatics is a techno-social issue

Organization of Nanoinformatics 2020 Roadmap The Blood

Workshop themes

- Data collection and curation
  - How researchers obtain and manage their own data, as well as how they discover data generated by others (database management, instrumentation, high-throughput data, nanometrology, semantic compatibility

Organization of Nanoinformatics 2020 Roadmap The Blood

Workshop themes

- Data collection and curation
- Tools and methods for data innovation, analysis, and simulation
  - Questions of data use such as data mining, semantic search, gap analysis tools, machine learning, visual analytics and workflow

Organization of Nanoinformatics 2020 Roadmap The Blood

Workshop themes

- Data collection and curation
- Tools and methods for data innovation, analysis, and simulation
- Data accessibility and information sharing
  - Deals with practical, cultural, legal and ethical aspects of data sharing such as proper annotation and attribution, cultural dynamics of data sharing across disciplines, barriers to data sharing, governance and regulation of data and IP, metadata standards and standards development
  - Holy Grail = federated system of interoperable databases

Organization of Nanoinformatics 2020 Roadmap The Guts

- Provided pilot project templates for breakout groups
  - **Problem description** – what is the problem to be addressed and why is it important?
  - **Current practice** – how is the problem currently being addressed (if at all), by whom, and what are the limitations to current practices?
  - **Proposed new approach** – what is the new approach to solving the problem and why is it time to use this approach now?
  - **Expected impact** – what impact would the new approach have and who would be impacted?
  - **Participants** – who is, or should be, involved?
  - **Budget requirements** – how much money is needed?
  - **Pilot metrics** – what are expected metrics or milestones to indicate success?

Organization of Nanoinformatics 2020 Roadmap

Proposed projects and progress-to-date

- Consortium for coordinating nanomaterial research data
  - Funding avenue identified by participants (National Science Foundation Research Coordination Networks)
  - Minimal funding, collaborative proposal submission to program
  - Perhaps NCIP Nanotechnology Working Group serves this purpose

Organization of Nanoinformatics 2020 Roadmap

Proposed projects and progress-to-date

- Data accessibility and information sharing
  - Deals with practical, cultural, legal and ethical aspects
  - ISA-TAB extension → ISA-TAB-Nano (addition of a material file specific for nanomaterials through community consensus building and testing) (ASTM E2909-13)

Organization of Nanoinformatics 2020 Roadmap

Proposed projects and progress-to-date

- Workshops focused on nanomaterials development using nanoinformatics
  - 2012 GreenerNano (GN12) Nanoinformatics Tools and Resources Workshop
  - Supported by the ONAMI Safer Nanomaterials and Nanomanufacturing Initiative (AFRL) and the NSF National Nanomanufacturing Network
  - Outcomes published in workshop report in Computational Science and Discovery
- Meta-ontology for cross-discipline, cross-sector information exchange
  - Nanoparticle Ontology – completed and in use
  - Metathesaurus to cross-navigate ontologies – still needed

Organization of Nanoinformatics 2020 Roadmap

Proposed projects and progress-to-date

- Minimum information requirements for data sharing (completeness and quality)
  - MinChar – bare bones but lacks detail to make comparable across studies, perhaps needs to be field-specific
  - NanoWG: Nanotechnology Data Curation Initiative
    - Series of 6 community developed papers
    - Data quality and completeness MS published in May, (*Marchese-Robinson et al., 2016*)

Organization of Nanoinformatics 2020 Roadmap

Proposed projects and progress-to-date

- Meta-crawler for mining nanotechnology repositories and open access sources
  - Several presentations to the NanoWG
    - Language from text, data from databases

- nanoSAR education and dissemination
  - Several presentations to the NanoWG
  - N4mics tool for visualizing data in the Nanomaterial-Biological Interactions knowledgebase (NanoHUB)

Organization of Nanoinformatics 2020 Roadmap

Proposed projects and progress-to-date

- Simulation resources and simulation challenge
  - Substantial funding required to perform this pilot in a comprehensive manner
  - Smaller funding could be identified to identify a meaningful component to focus on

Organization of Nanoinformatics 2020 Roadmap

Communication and Assessment Guidelines for the Roadmap

- Emphasize literacy and develop critical thinking
- Develop and use real-life data examples
- Stress conceptual understanding rather than mere application of procedures
- Foster continuous improvement and active discussions
- Use technology for developing conceptual understanding and for analyzing and sharing information (modeling and simulation, databases, etc.)
- Use assessments to improve and evaluate the efficacy and impact of these activities

Organization of Nanoinformatics 2020 Roadmap

Bibliography for the Roadmap

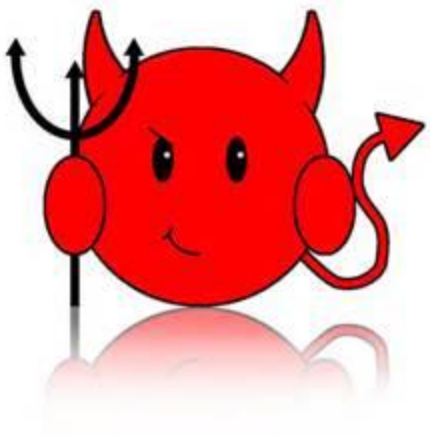
- Conference proceedings that contributed to the workshop outcomes (NI 2020 Roadmap)
- Articles – some proceedings, some reports, some primary literature
- White papers
- Reports

Organization of Nanoinformatics 2020 Roadmap

Lessons learned from the 2010 workshop

- Meetings and conversations had been ongoing with diverse groups for years – the timing was right
- Homework given prior to the workshop benefited discussions
- Taking inventory of what we have already and ongoing activities was critical – needed to leverage resources
- Want to gain community consensus but not at the loss of roadmap integrity, so…

Invitation to Play Devil's Advocate



Definition: *A **devil's advocate** is someone who, given a certain argument, takes a position they do not necessarily agree with, for the sake of debate or to explore the thought further.*

By playing devil's advocate, you can help us:

- To avoid **group think**
- To engage all in an argumentative **discussion process**
- To **identify weaknesses** in a position/stance
- To **identify alternatives** to the accepted norm