CEINT NanoInformtics Knowledge Commons (CEINT-NIKC)
Building Research Tools for Nano EHS

Greg Lowry, Sandra Karcher, Yuan Tian,
Jeanne VanBriesen, Christine Hendren, Mark Wiesner

Carnegie Mellon University, Duke University
Department of Civil and Environmental Engineering

www.ceint.duke.edu

Center for the Environment Implications of Nanotechnology

Core Institutions: Duke, CMU, Stanford, Howard, Kentucky, Va Tech

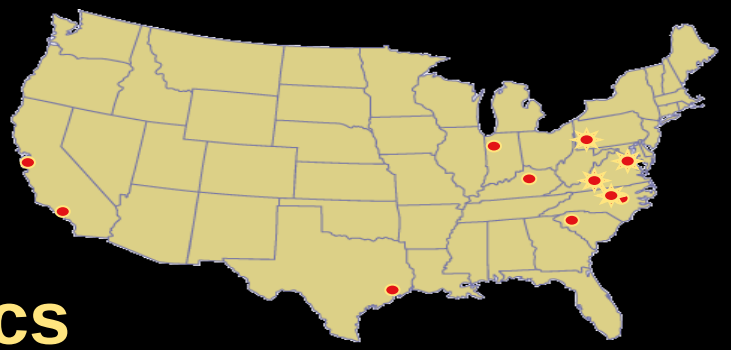
$30M from NSF + EPA

10-years (currently in yr 7)

43 faculty, >130 Students/P-docs

Interdisciplinary

- **Env. Eng., Geochemistry, Public Policy, Chem E., Mat Sci., Chemistry, Ecology, Toxicology**

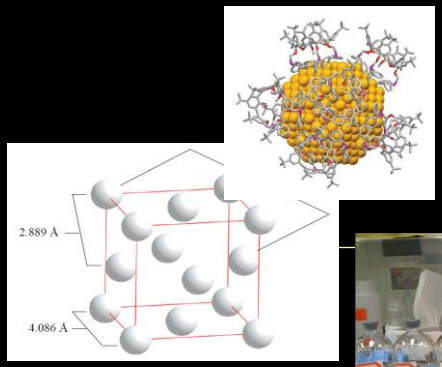


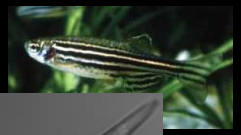
Goal:

Elucidate the relationship between the vast array of nanomaterials and properties to their environmental and human health risks

CEINT
Center for the Environmental Implications of NanoTechnology

Process to Achieving this Goal



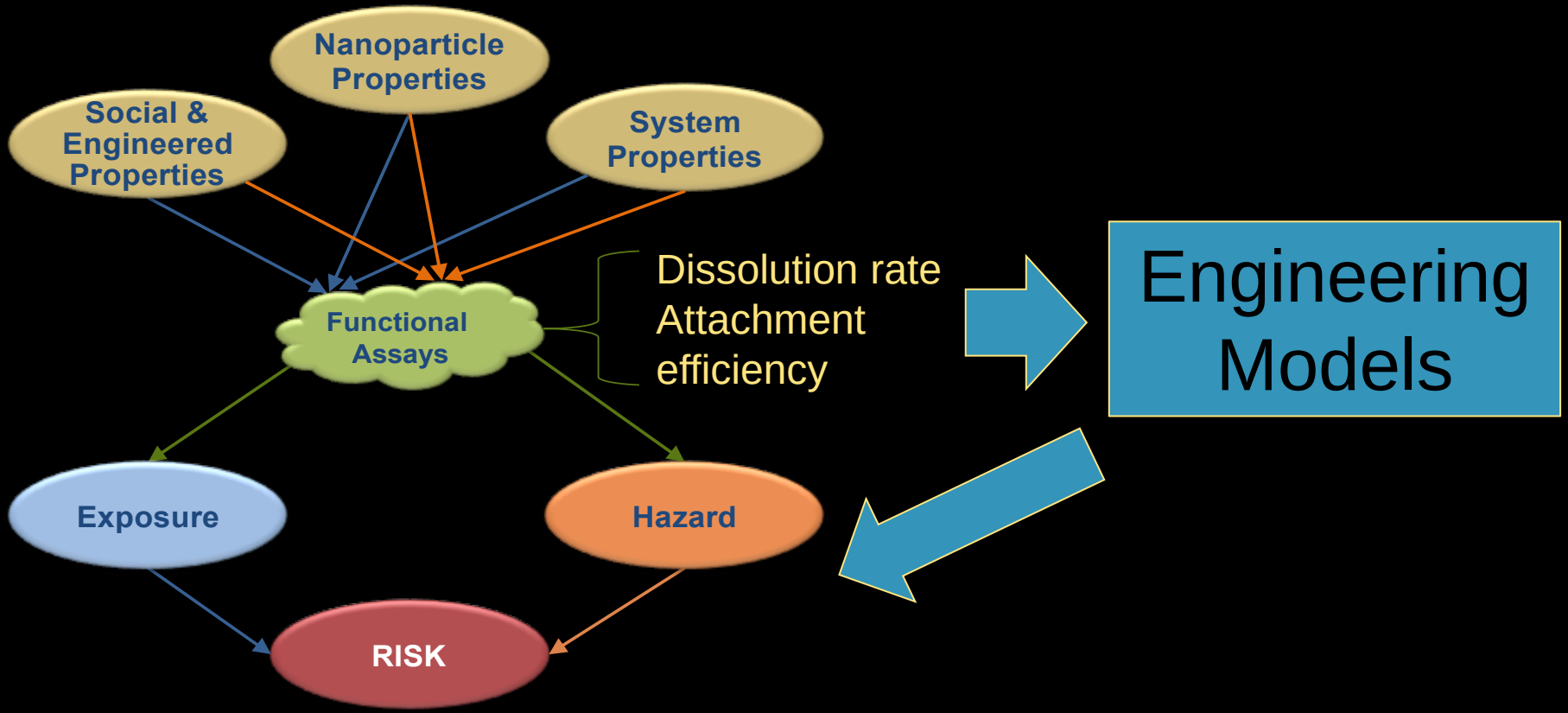


Increasing Scale

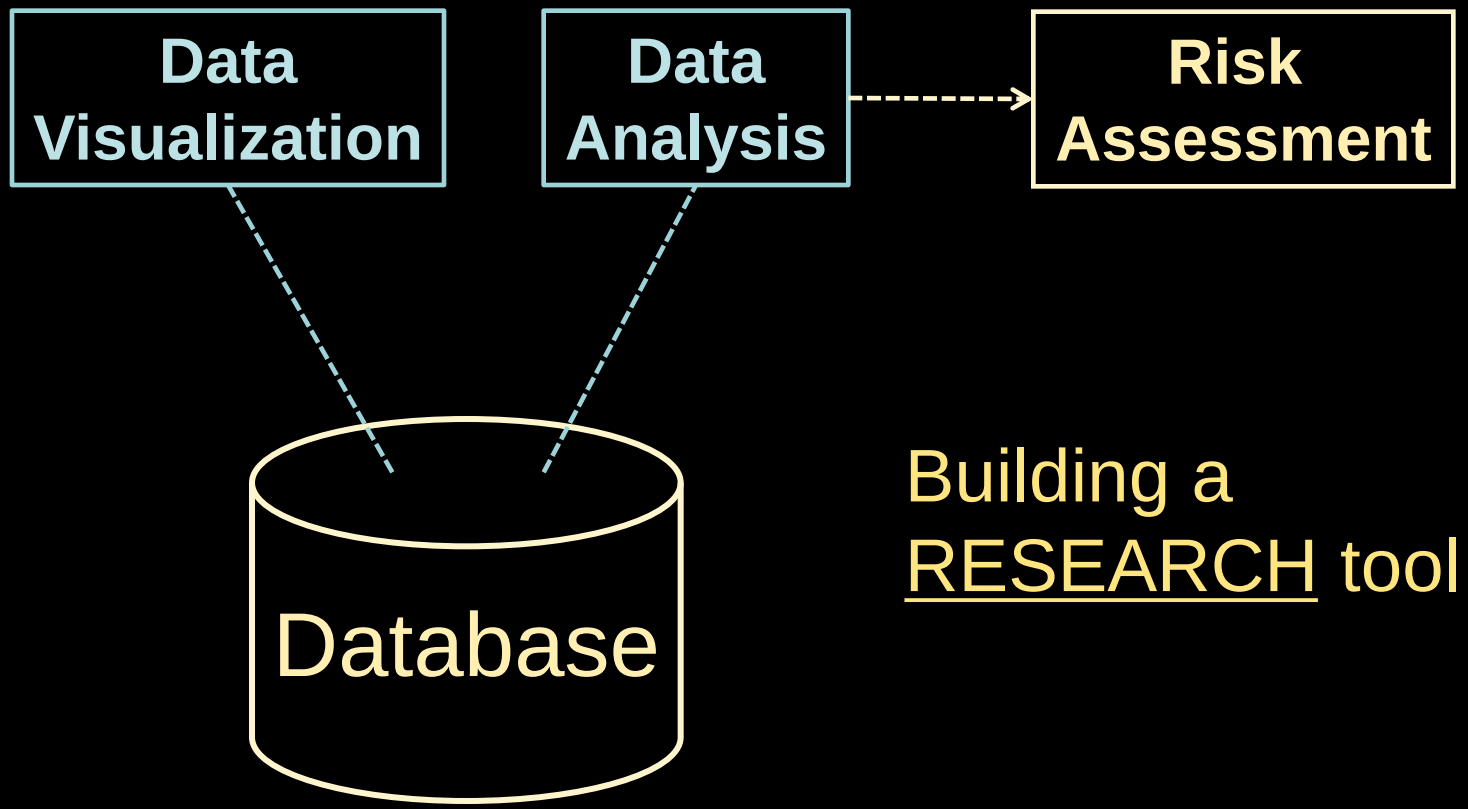
Increasing Complexity

Ag, Au, CuO, Ni, ZnO, TiO_2, and CeO_2 particles, and CNT/C_{60}

CEINT Approach to Managing Complexity



Goal of CEINT-NIKC



Building a RESEARCH tool

Database Design and Approach

1) Structure for storage
2) Protocols for populating
3) Key fields for querying

- SQL (MSFT Access)
- Develop and document
- Use key fields to organize, sort, and pull subsets of our data together

Information Flow

- an **Experiment** or manufacturing process
- occurs at a **Location**
- in a **System**
- of **Matrix** (e.g., soil, water, plant, etc.)

*at specific **time** points:*

- an **Action** happened (take something out, add something, or measure something in-situ)
- following a set of **Methods** or protocols
- resulting in a measurement or observation of a specific **Parameter**

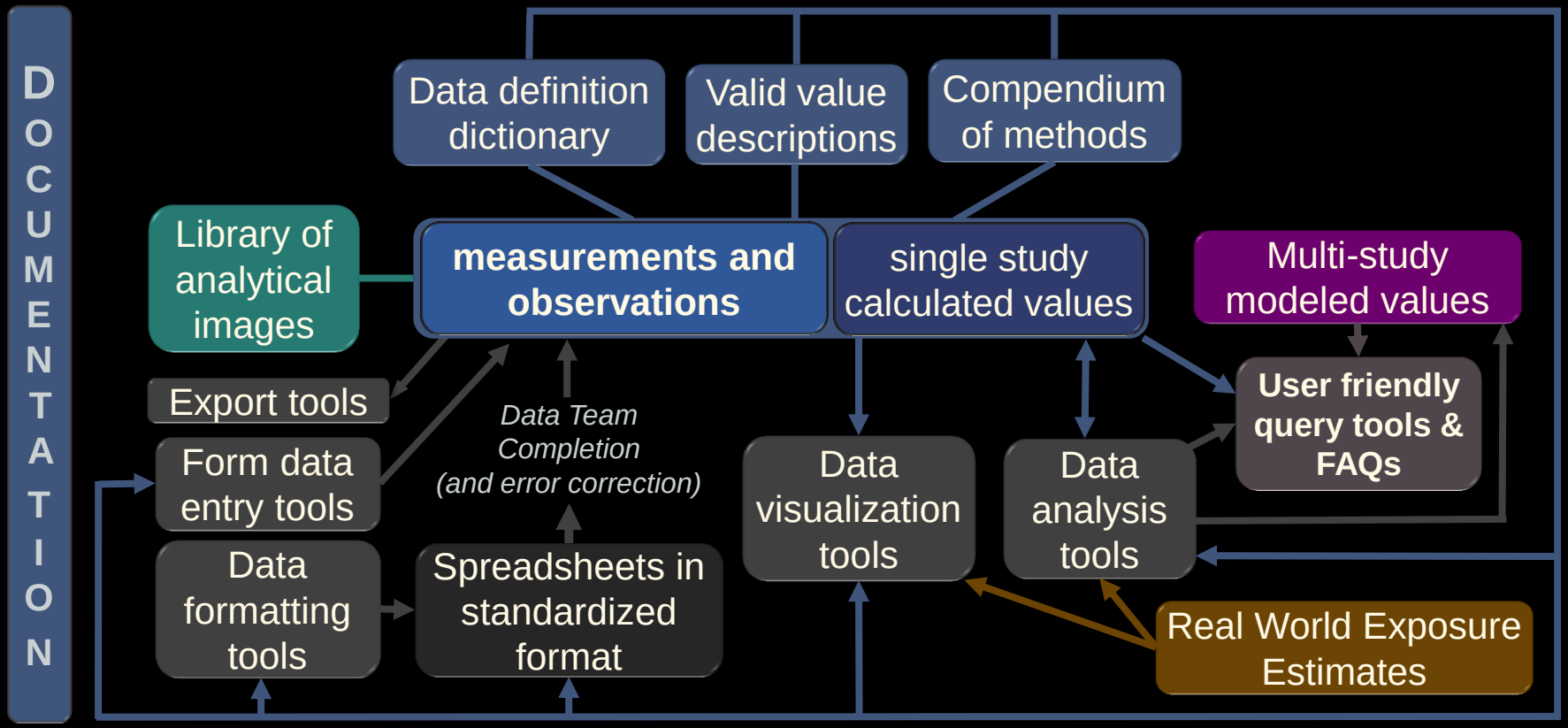
after the experiment has be completed, typically:

- we **calculate** something following a method or protocol

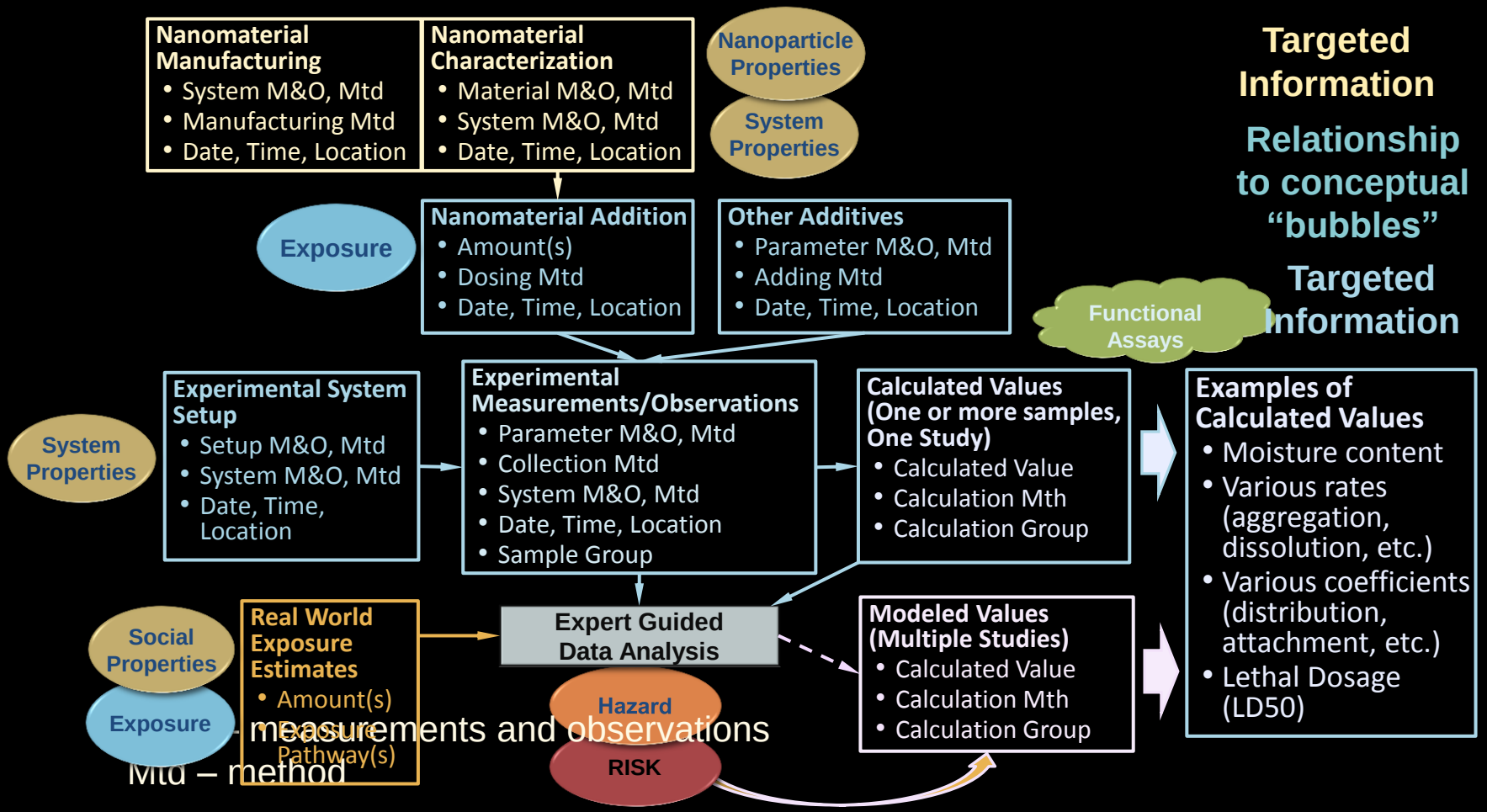
Targeted Information

- Nanomaterial characterization
  - Associated metadata
- System characterization
  - Associated metadata
- Nanomaterial dosing information
- Experimental methods
- Experimental results
- Calculated values

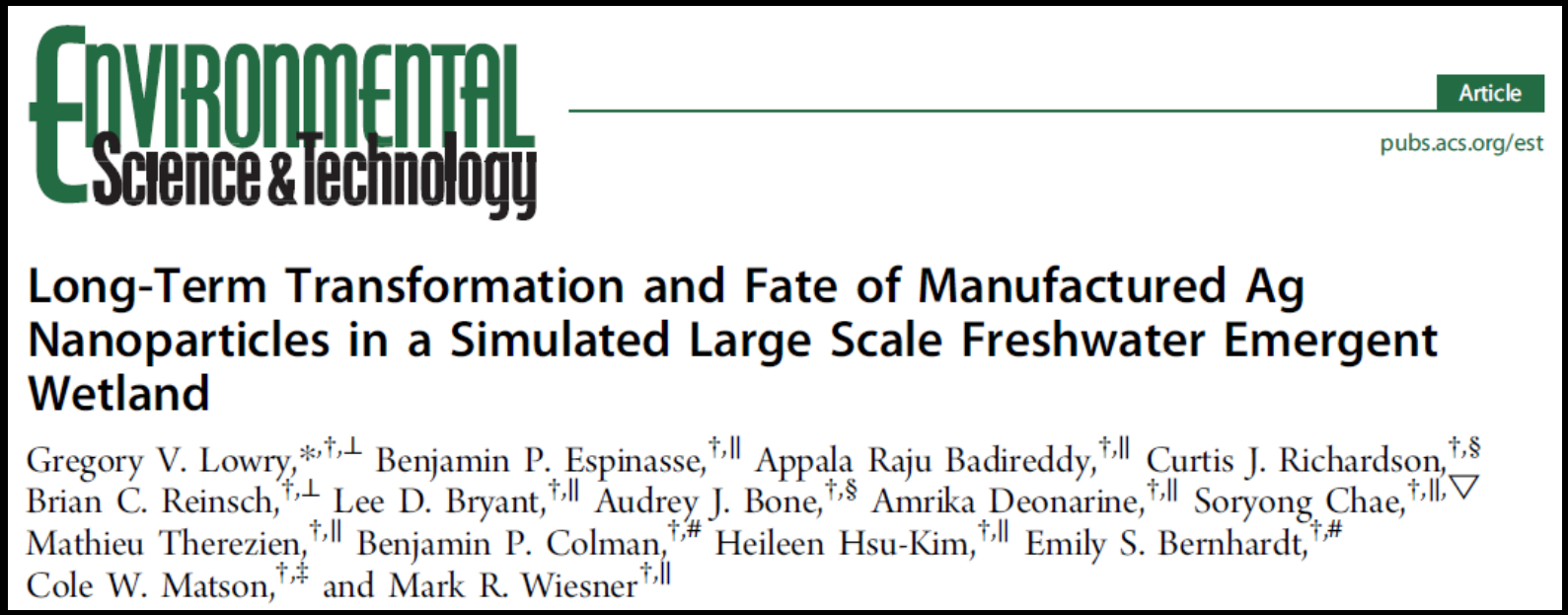
Components of CEINT-NIKC



Alternative View of M&O Plus



Using Data From



Environmental Science & Technology

Article

pubs.acs.org/est

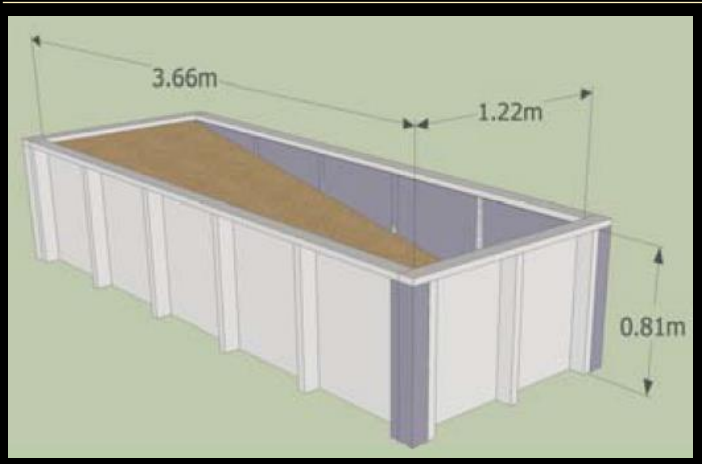
Long-Term Transformation and Fate of Manufactured Ag Nanoparticles in a Simulated Large Scale Freshwater Emergent Wetland

Gregory V. Lowry,[*,†,⊥] Benjamin P. Espinasse,[†,∥] Appala Raju Badireddy,[†,∥] Curtis J. Richardson,[†,§] Brian C. Reinsch,[†,⊥] Lee D. Bryant,[†,∥] Audrey J. Bone,[†,§] Amrika Deonarine,[†,∥] Soryong Chae,[†,∥,▽] Mathieu Therezien,[†,∥] Benjamin P. Colman,[†,#] Heileen Hsu-Kim,[†,∥] Emily S. Bernhardt,[†,#] Cole W. Matson,[†,‡] and Mark R. Wiesner[†,∥]

dx.doi.org/10.1021/es204608d | *Environ. Sci. Technol.* 2012, 46, 7027–7036

CEINT Center for the Environmental Implications of NanoTechnology

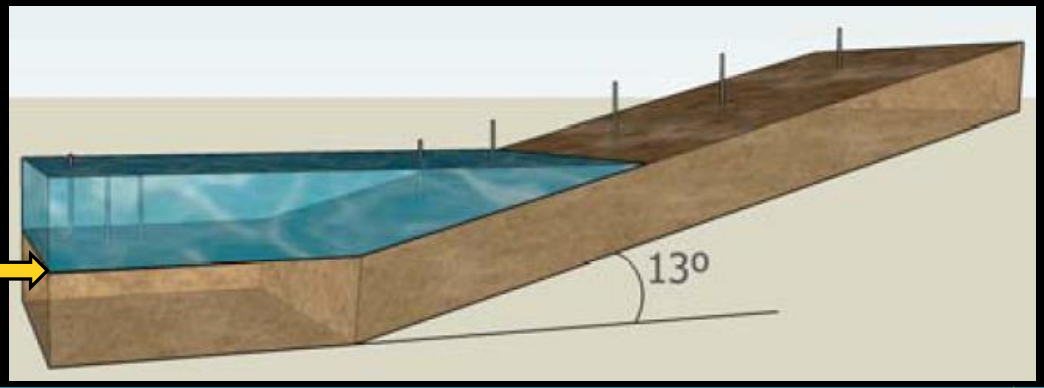
Experimental Setup



- One mesocosm dosed in soil compartment
- One mesocosm dosed in water compartment

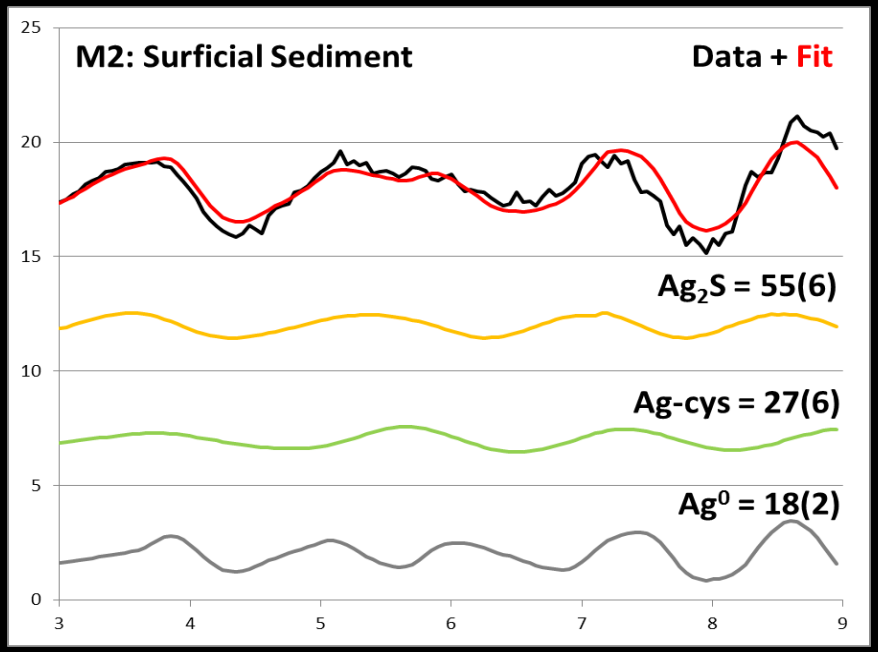
- DO above SWI
- Cores
  - 18
  - 4 depth intervals

Surface Water Interface (at 0)



AgNPs Sulfidize in the Environment

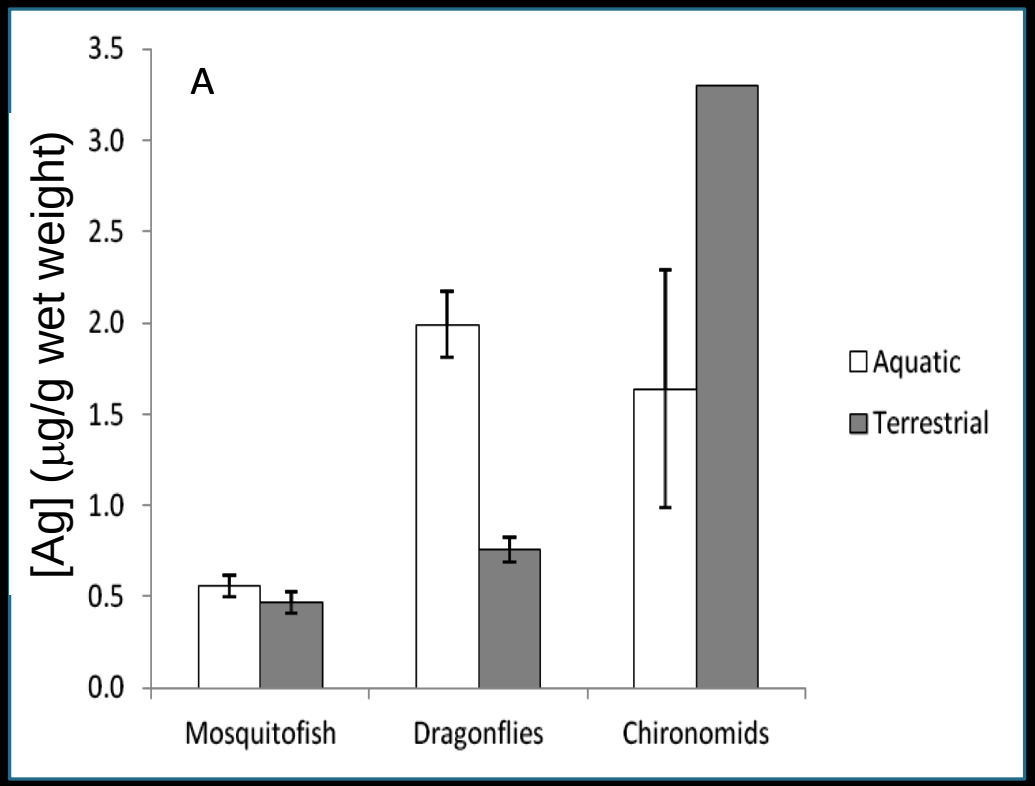
Ag Speciation in Aquatic Sediments



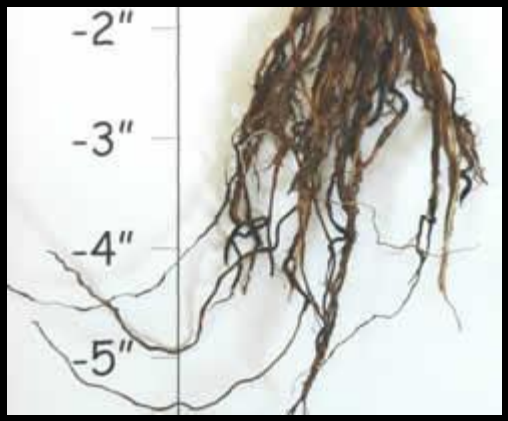
Lowry et al., ES&T 46 2012 (13), pp 7027–7036

CEINT
Center for the Environmental Implications of NanoTechnology

Ag Bioavailability in Mesocosms



Roots (20 mg/kg)



Lowry et al., ES&T 46 2012 (13), pp 7027–7036; Colman et al., (in prep)

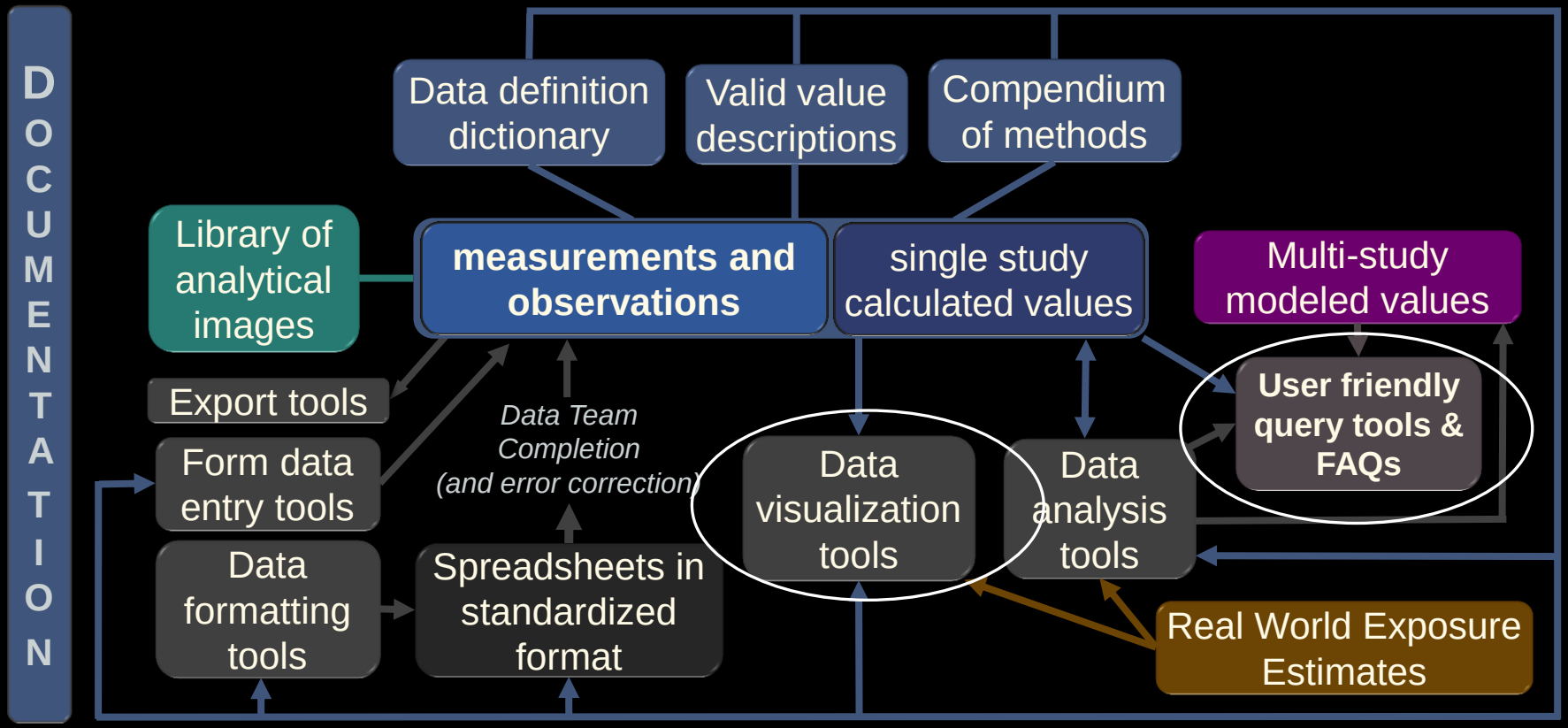
CEINT
Center for the Environmental Implications of NanoTechnology

Summary Statistics on DO

- Find average dissolved oxygen concentration just above the surface water interface
  1) Pull the relevant records

Location Group	Location Group Number	Sample Beginning Depth	Sample Ending Depth	Depth Unit	Sample Matrix	More Specific Information about the Sample Matrix	Parameter of Interest	Measured Value	Parameter Unit
mesocosm	1	-4.2	-4.2	millimeter	water	surface water interface	dissolved oxygen	208.4	micromolar
mesocosm	1	-3.2	-3.2	millimeter	water	surface water interface	dissolved oxygen	202.8	micromolar
mesocosm	1	-2.1	-2.1	millimeter	water	surface water interface	dissolved oxygen	203.2	micromolar
mesocosm	1	-1.1	-1.1	millimeter	water	surface water interface	dissolved oxygen	191.8	micromolar
mesocosm	2	-6.0	-6.0	millimeter	water	surface water interface	dissolved oxygen	221.8	micromolar
mesocosm	2	-5.0	-5.0	millimeter	water	surface water interface	dissolved oxygen	216.1	micromolar
mesocosm	2	-4.1	-4.1	millimeter	water	surface water interface	dissolved oxygen	200.5	micromolar
mesocosm	2	-3.0	-3.0	millimeter	water	surface water interface	dissolved oxygen	202.1	micromolar
mesocosm	2	-2.0	-2.0	millimeter	Water	surface water interface	dissolved oxygen	185.2	micromolar
mesocosm	2	-1.1	-1.1	millimeter	Water	surface water interface	dissolved oxygen	157.8	micromolar

Components


DOCUMENTATION
Data definition dictionary
Valid value descriptions
Compendium of methods
Library of analytical images
measurements and observations
single study calculated values
Multi-study modeled values
Export tools
Form data entry tools
Data Team Completion (and error correction)
Data visualization tools
Data analysis tools
User friendly query tools & FAQs
Data formatting tools
Spreadsheets in standardized format
Real World Exposure Estimates

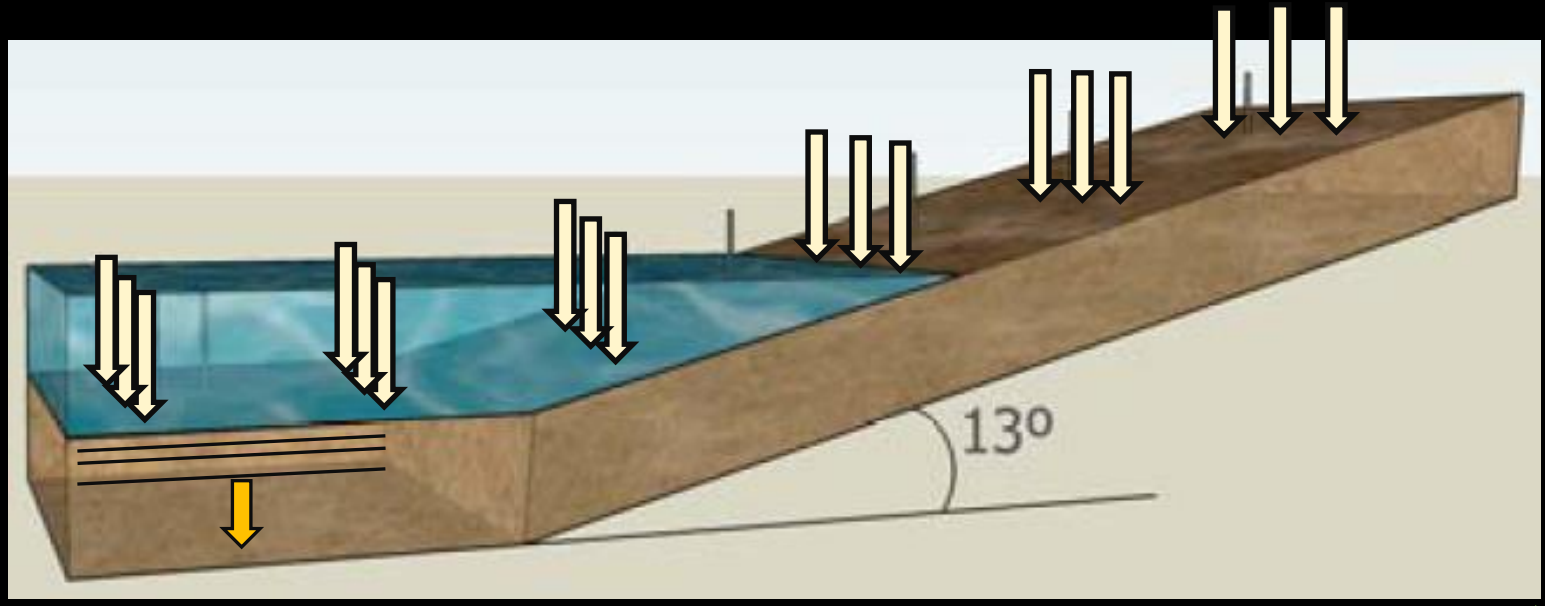
User friendly query tools & FAQs

- Easily get answers to predefined questions
  - Does NP size determine fate or effects?
  - Does NP dissolution rate determine biouptake?
  - Does natural organic matter concentration determine toxicity?
  - Does NP coating type determine toxicity?

These questions are moving targets and will update as more knowledge is gained!

GIS Visualization - Background

- Mass of silver in sediment
  - 3 by 6 grid (18 cores)
  - Spit into 4 depth intervals



GIS Visualization

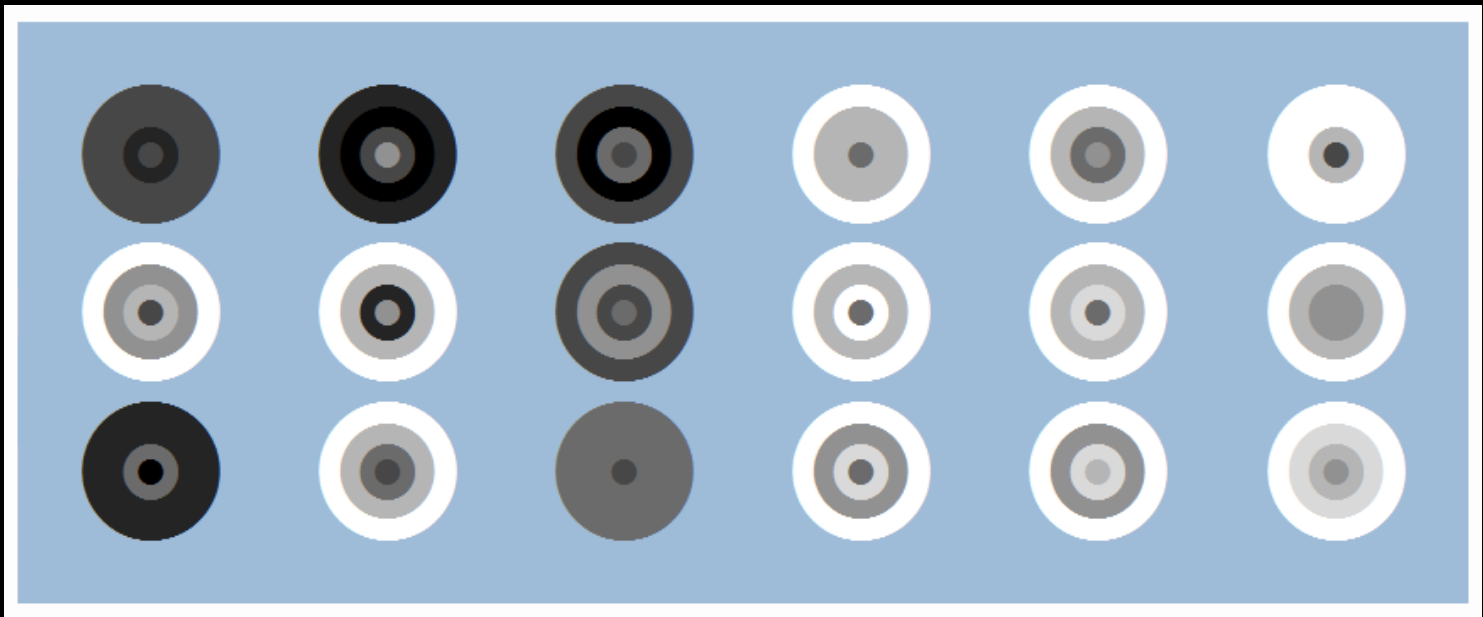
- Query the database
  - Data Source of GVL2012LongTerm
  - Matrix of soil or sediment
  - Parameter label of silver
  - Elapsed time > 530 days
  - Units of milligram

Query the Dataset

Data Source	Location Group	Location Group Number	Elapsed Time	X Coordinate	Y Coordinate	Beginning Depth	Ending Depth	Depth Unit	Sample Matrix	Parameter of Interest	Parameter Unit	Measured Value
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	0	1	centimeter	sediment	silver	milligram	27
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	1	2	centimeter	sediment	silver	milligram	10.7
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	2	4	centimeter	sediment	silver	milligram	6.4
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	4	22	centimeter	sediment	silver	milligram	0
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	0	1	centimeter	sediment	silver	milligram	19.1
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	1	2	centimeter	sediment	silver	milligram	6.9
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	2	4	centimeter	sediment	silver	milligram	4.5
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01773	4	22	centimeter	sediment	silver	milligram	0
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01774	0	1	centimeter	sediment	silver	milligram	12.5
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01774	1	2	centimeter	sediment	silver	milligram	32.4
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01774	2	4	centimeter	sediment	silver	milligram	11.3
GVL2012Long Term	mesocosm	1	580.8	-78.9822	36.01774	4	22	centimeter	sediment	silver	milligram	0

Water Dosed Mesocosm

- Circle diameter increases with depth
- Darker shade indicates more silver mass



water side soil side

Summary and Forward Looking

- Building a research tool, not just a repository
  - But, it will be interoperable with materials databases, e.g. NR
- Data curation in a meaningful way is *excruciating*
  - Need to populate database for meaningful analysis
- Key questions drive database structure and data collection
  - Chicken and egg problem
- Compendium of methods is needed
- Working to make data entry easier for users
  - Key fields depend on key questions
- Working on data analysis and data visualization tools