Leveraging an Integrated NanoAg Dataset:
A Pilot Collaboration Project Between CEINT, the Nanomaterial Registry, and NanoHUB

Nanomaterial Registry, NanoHUB, CEINT

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CEINT
Center for the Environmental Implications of NanoTechnology

NANOMATERIALREGISTRY

nanoHUB.org

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Agenda

- Basis for collaboration
- CEINT perspective
  - Brief overview of mission, organization and activities
  - Internal approach to data integration
- Pilot project
  - Scope – subset of complex published nanoAg papers
  - Roles for each organization
- Group discussion
  - Reactions? Short and long-term possibilities?
  - List of specific data structuring/curation questions

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Basis for Collaboration

This collaboration was started based on the idea that all three of our organizations can benefit from leveraging one another's core competencies to further our individual and collective goals.

Who	Have	Want
Nanomaterial Registry	• Data architecture for nano physicochemical characteristics, environmental study data and toxicity data • Authoritative, repeatable curation process • Links to ontology and ISA-TAB Nano Standards • Curated sub-set of CEINT silver dataset in SQL and Excel	• User community • A data subset that will allow proof-of-concept for trend analyses
NanoHUB	• Established user community • Database creation skills and bandwidth to take on a specific project	• Increased data focus • A data subset that will serve as proof-of-concept for linking curated data to simulation tools and models
CEINT	• Integrated silver dataset • Parameters that will describe: o Reference materials o Reference systems o Reference scenarios	• Custom database to capture CEINT data and metadata that: o Allows analyses that would answer specific research questions o Maps to NR/NPO terminology
TEAM	• A dataset • Established terminology for parameters and meta-data • Database expertise	• Clear project scope • Database for CEINT nano-Ag data

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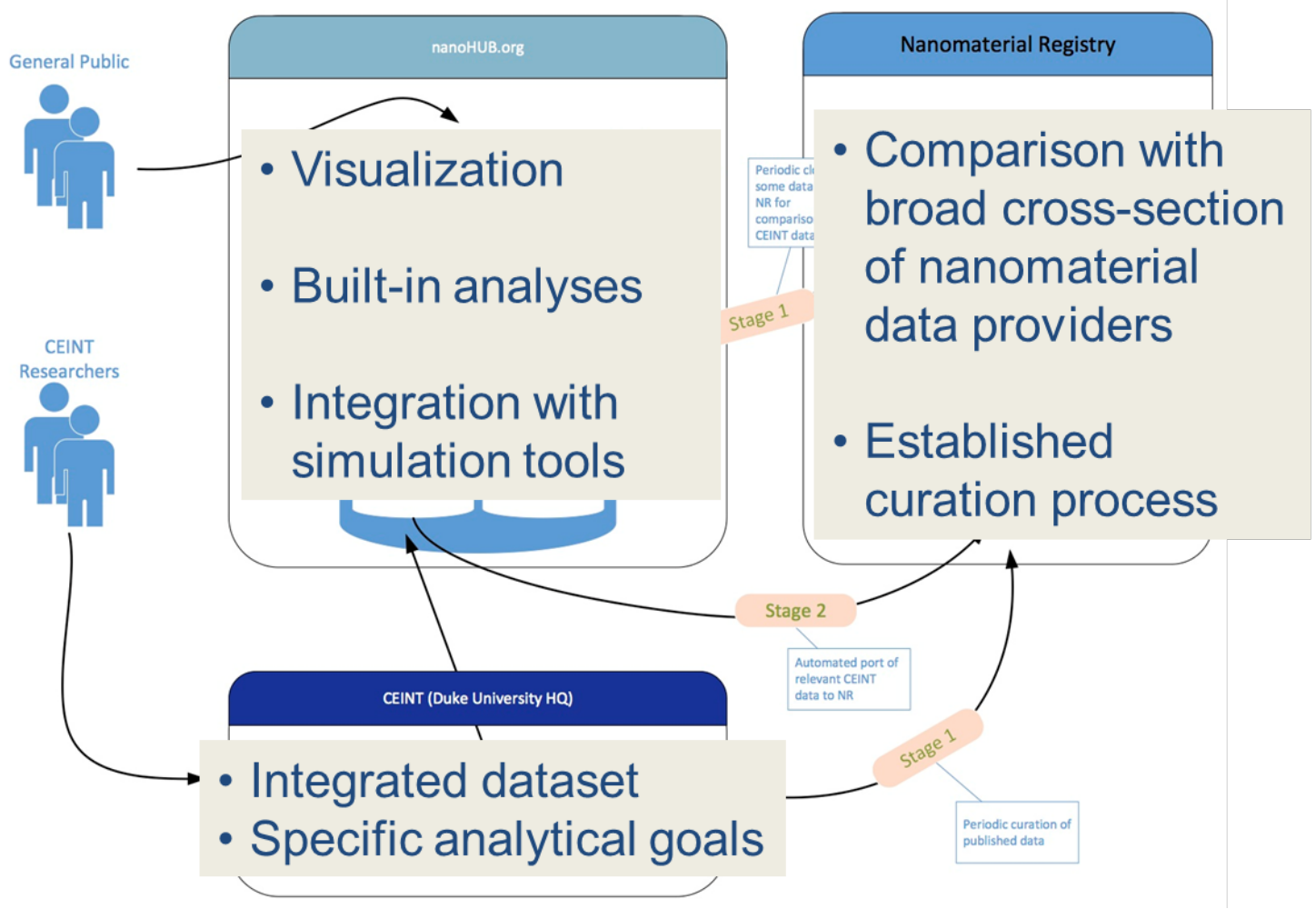
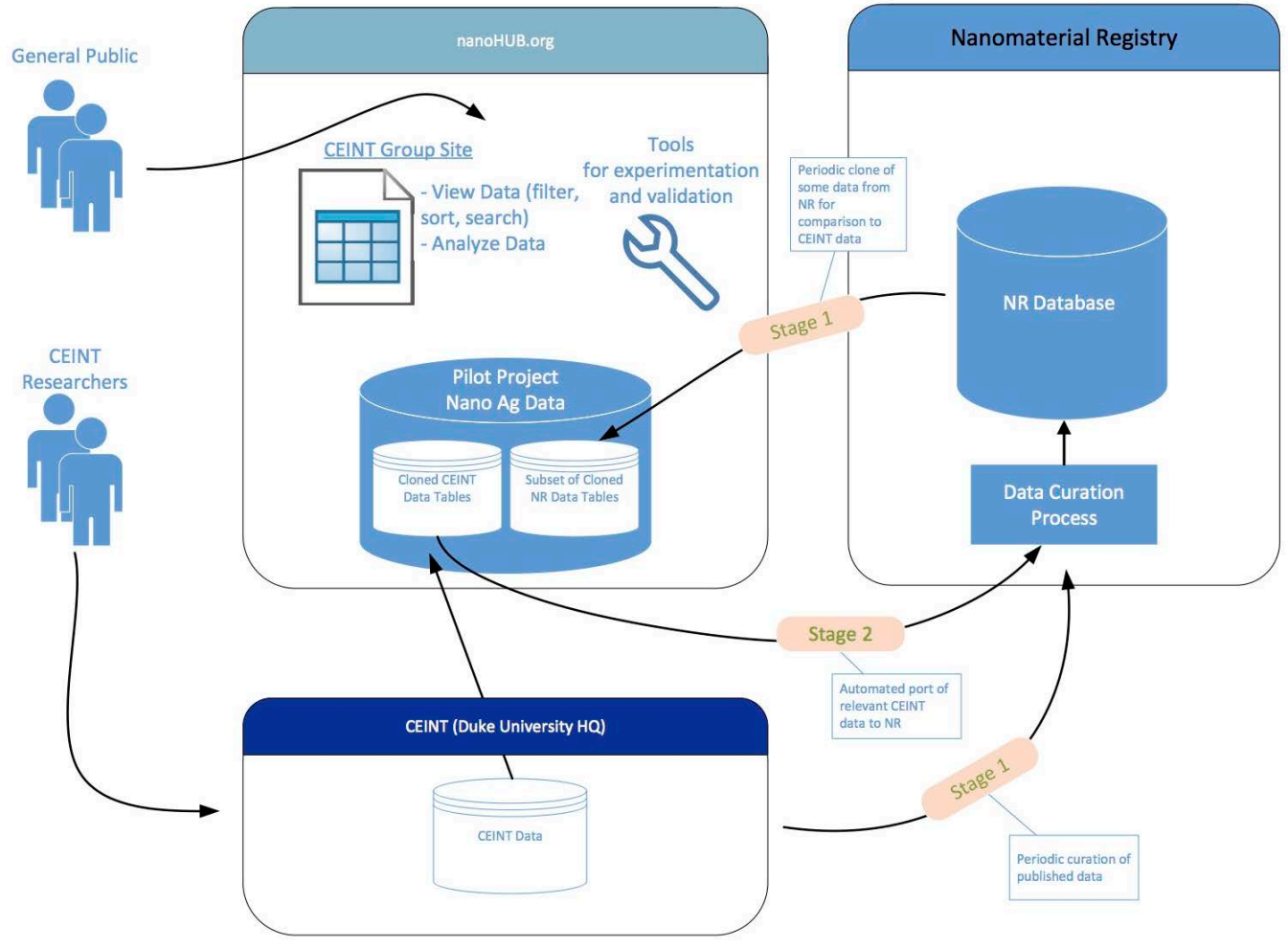
Schematic of Collaborative Roles (1)



Schematic of Collaborative Roles (2)



Group Discussion

- There are many deceptively simple fundamental questions that are non-trivial and could benefit from all of our minds together.
- Could we utilize the wiki as a discussion board for specific questions?
- Perhaps we can also tackle one at a time, time permitting, during standing meetings

Fundamental, non-trivial question #1

What defines an individual material, and an individual record, in a DB?

Record

- Document of origin?
- [Material + Endpoint] Combination?
- Arbitrary with respect to content, based on tracking curation efforts?

Material

- Product?
- Lot? (each manufacturer may define differently)
- [Core Composition + Coating] Combination?

Starter List of Example DB Questions

(1). AEROXIDE® P25 can be found in many toxicity papers and already enjoys 2 NR numbers. As with PCC data, what are the options of organizing multiple references to toxicity and ecotoxicity data originating from a single NR number ?

(2). AEROXIDE® P25 can be found in many toxicity papers and already enjoys 2 NR numbers. As with PCC data, what are the options of having multiple references to toxicity and ecotoxicity data originating from a single NR number ?

(3). Many colleagues have used commercial materials that exist today and have been characterized today, but were not characterized then using today's techniques. How should "valid" historical data be graded using the "compliance score?"

(4). How do we design the NR to follow guidelines for "robust summaries" for its summaries of toxicity and ecotoxicity data?

(5). When someone does make a comment, what are the procedures to follow in terms of acknowledgement and making changes in the record ?

(6). Instances of characterization → Europe is developing more of them, so is it time to define "minimum instance of characterization"?


Questions?