

Metadata Requirements and Projects for Nanomaterial Characterization

Martin Fritts

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Advanced Technology Program

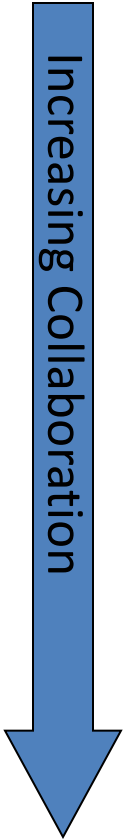
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Nanomaterial Characterization

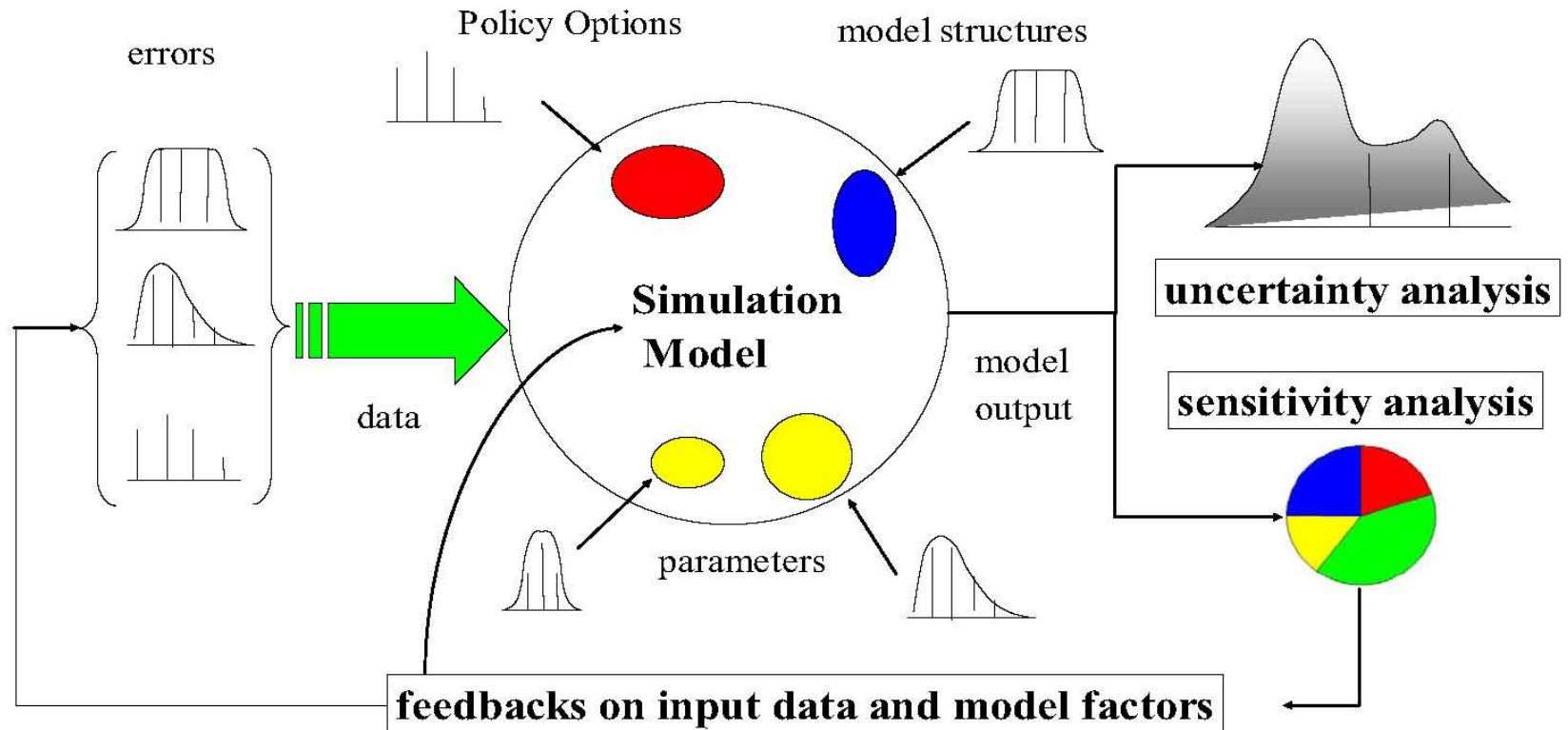
- Physico-chemical properties
- In vitro
- In vivo
 - Standard Protocols
 - Sample Preparation
 - Interlaboratory Studies
 - Routes of Exposure
- With Genomic, Proteomic Data
- In silico experiments
- SARS
- Personalized Medicine

caNanoLAB
FDA, NIST
ILS: ASTM, IANH, ...
NPO
NIEHS... caBIG WG
Nano-TAB (ISA-TAB)
CSN
ACTION-Grid

Increasing Collaboration



Design Sensitivity Analysis and Optimization



From: "Sensitivity Analysis", Andrea Saltelli, European Commission,
Joint Research Centre, Ispra,
Presented at Piacenza, May 14-15 2009

Informatics Needs

The need for a federated informatics infrastructure with layered access control for public and private data

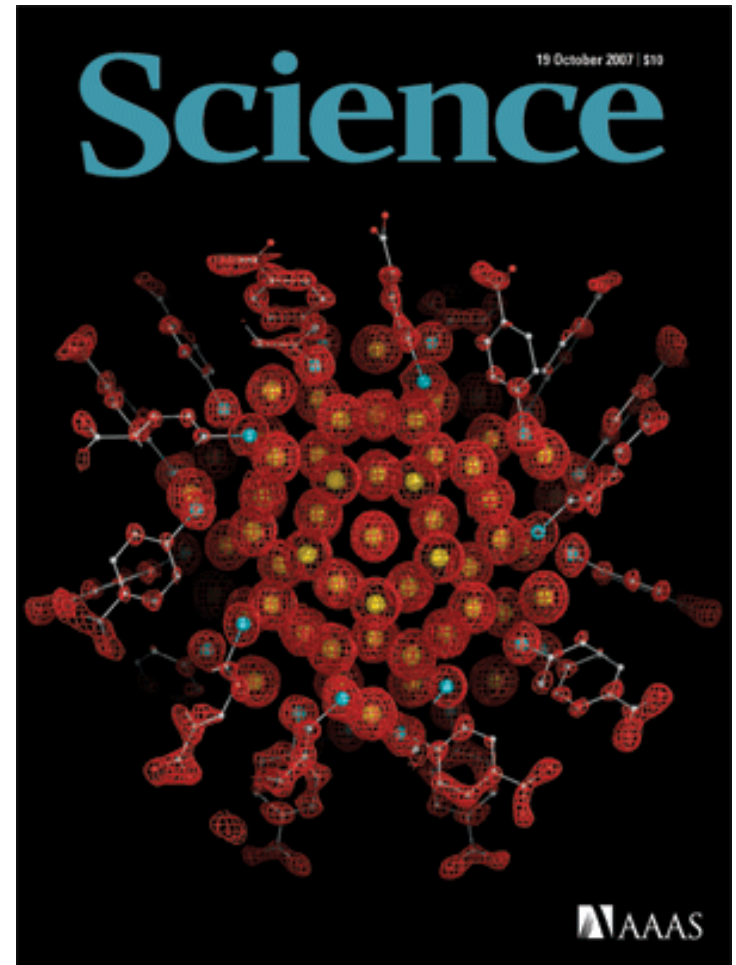
The need for measures of error and uncertainty in the data

The need for semantic search

- Ontology development and mapping
- Standards (Nano-TAB)
- Advanced search
- Search based on structural motifs of interest
- Nanomaterial registry

The need for coupling uncertainty analysis and sensitivity analysis using predictive models

The need to develop, share and validate structural, computational and predictive models



Summary

The need for collaboration in nanotechnology may be best summarized in analogy with the parable of the blind men and the elephant.

- Input from scientists in different disciplines is needed to develop nanotechnology applications (particularly with respect to their activity - and reporting error and uncertainty)
- Each disciplines may examine different aspects of the structure of nanomaterial using their preferred tools (“If you test with one technique you are inevitably wrong”)
- Communication about both structure and activity are hindered by lack of communication of what “they mean” (i.e., lack of semantics)
- They need a shared conceptual, analysis, and simulation models through which to reference and annotate their observations and to formulate structure-activity relationships
- Intelligent design is not possible without shared models and good communication among disciplines (especially for EHS risk analysis and mitigation)