Role of Modeling and Simulation in Materials Science Education and Research

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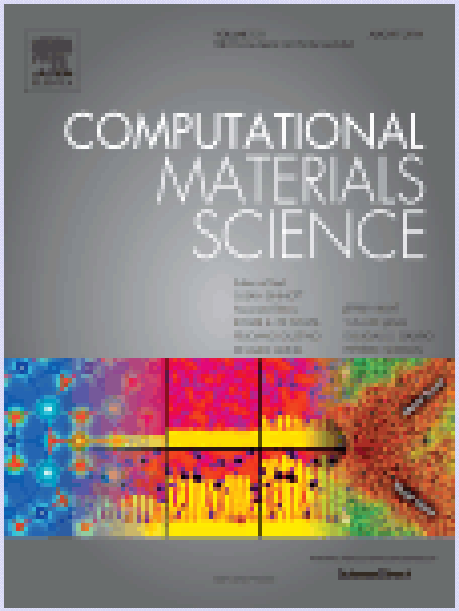
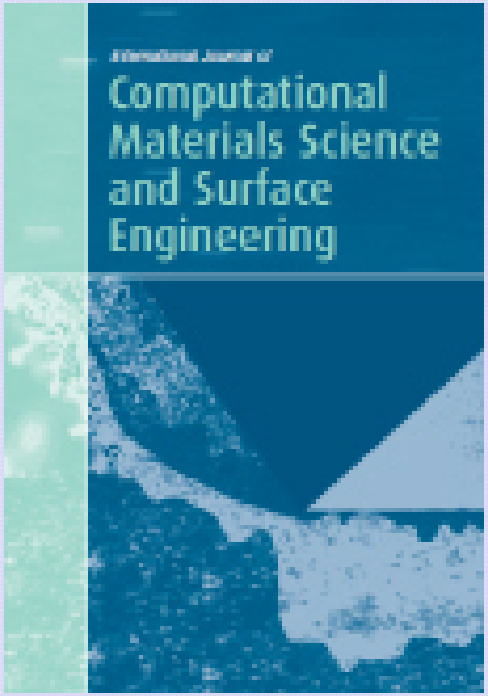
This talk is dedicated to the memory of Asst. Professor Yenerr Kuru

Synopsis

- *The design of materials guided by computation is expected to lead to:*
  - ✓ *Discovery of new materials,*
  - ✓ *Reduction of development time and cost,*
  - ✓ *Rapid evolution of new materials into products.*
- *There are journals specifically dedicated to this field of study.*
- *Significant resources are invested in this effort.*





Software for Modelling and Simulation in Materials Science

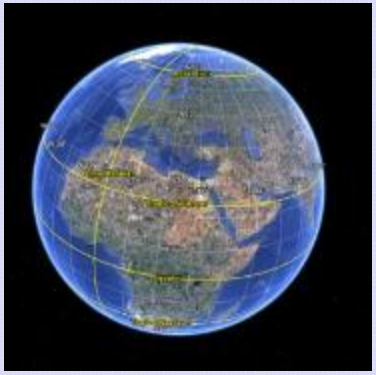
- Prediction of the arrangement of an ensemble of atoms through "energy minimization" (DFT, MD.)
- Modelling response of materials to mechanical, thermal or electrical impulses (FEM, FD)
- Prediction of phase diagrams, microstructures after equilibrium and non-equilibrium cooling.
- Simulation of diffusion-controlled reactions: sintering, interdiffusion, hard-coatings…
- Modelling concurrent nucleation, growth, coarsening and dissolution of precipitates
- Prediction of diffraction images …

- *Prediction: computational techniques will make classical theory and laboratory work "obsolete". (?)*

- *Sometimes computer simulation results are termed "data" and simulation runs are termed "experiments".*
- *I will discuss some basic concepts relevant to such efforts.*

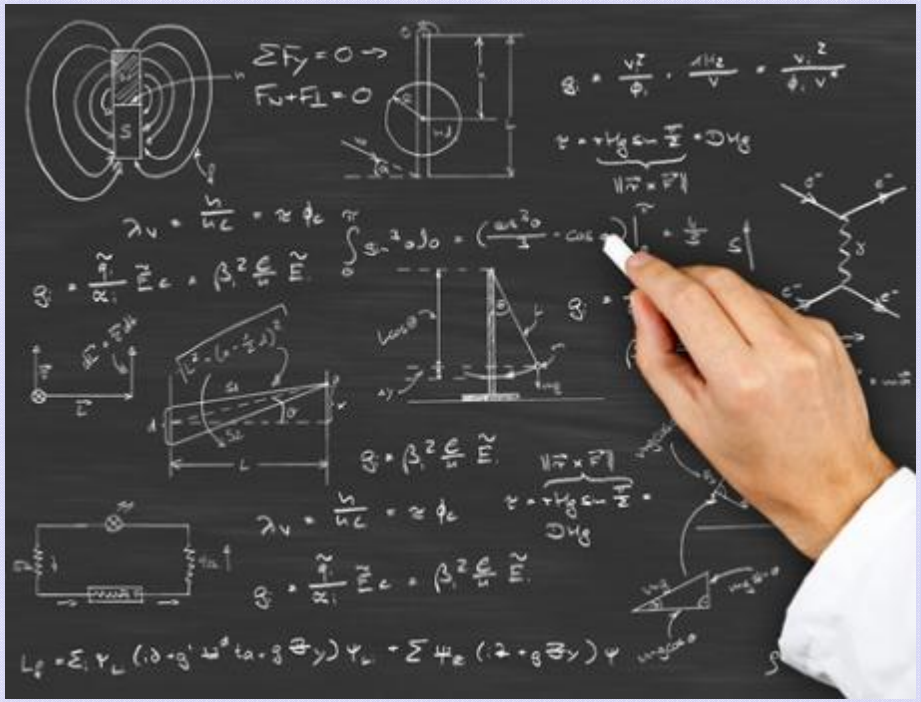
Definitions

Model



- ✓ a miniature representation of something;
- ✓ a description or analogy used to help visualize something that cannot be directly observed;
- ✓ *a system of postulates, data and inferences presented as a mathematical description of an entity or state of affairs.*

Modeling: a cognitive activity in which we think about how objects of interest behave and how to construct models to describe such behaviour.

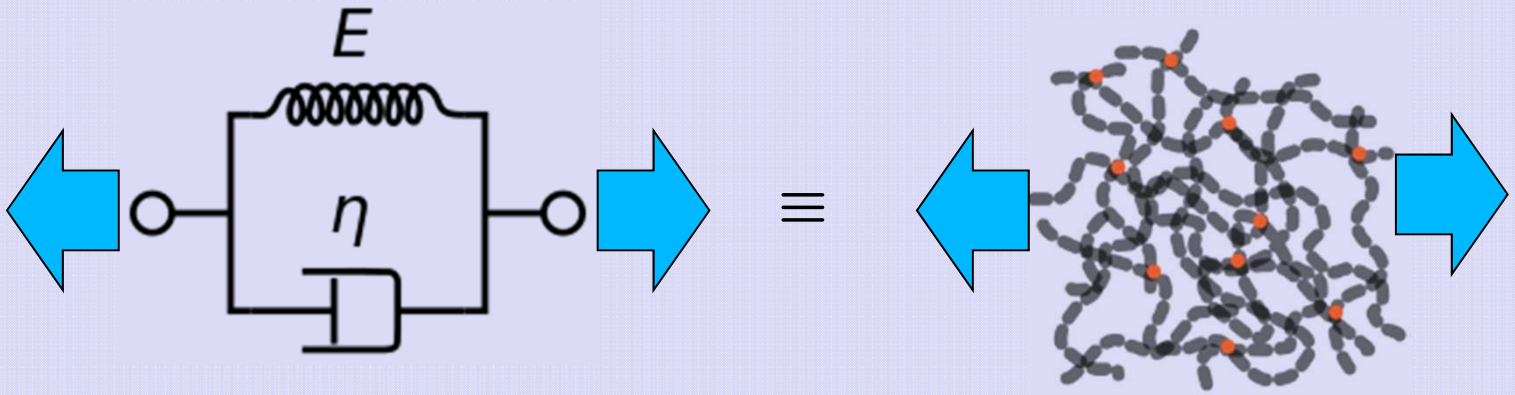


Cognition: "the mental action or process of acquiring *knowledge and understanding* through thought, experience, and the senses. (wikipedia)

- Mathematical-physical (M-P) models : *idealized* or approximate *representation of the behavior of real devices and objects* in mathematical terms.
  - Idealization: a deliberate simplification of complicated systems with the objective of making them more tractable.
    - ✓ Aristotelian idealizations: 'stripping away all properties from the system that are not relevant to the problem at hand. →a limited set of properties in isolation.
    - ✓ Galilean idealizations: substituting simpler phenomena* into the system to replace of the actual (complicated) ones (*point masses moving on frictionless planes*).
  - Almost all modern models are combinations.

**Substituting a simpler mathematical equation is termed approximation.*

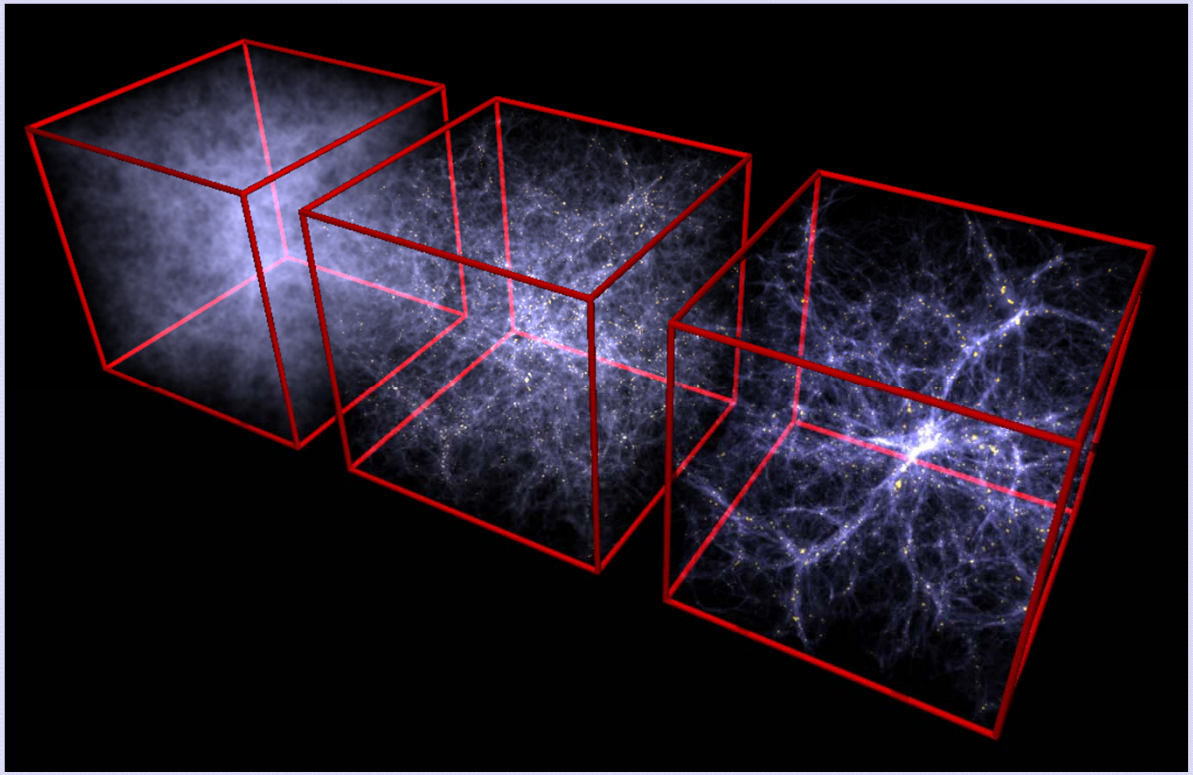
- Analogical models: Describing the system of interest through analogy to a simpler system with similarities in the relevant properties.



  - ✓Formal analogy: Two items are related by formal analogy if they are both interpretations of the same formal calculus (swinging pendulum / oscillating electric circuit; simple harmonic oscillator)

- Phenomenological models: models which only represent observable properties of the target systems and refrain from postulating hidden mechanisms.

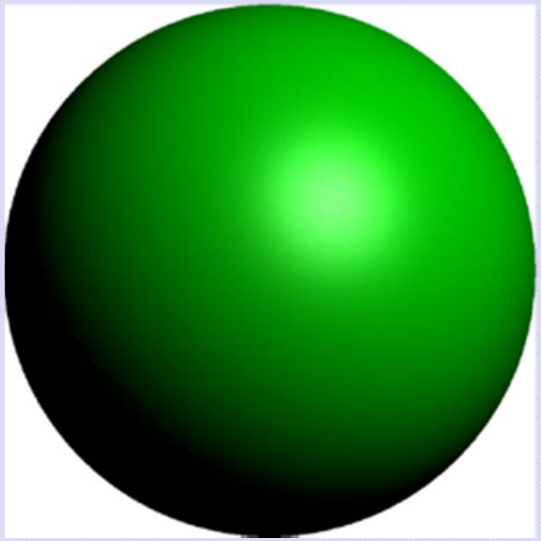
- Simulations are characteristically defined as "dynamic" models, i.e. models that involve the variation of one or more variables during the simulation.
  - ✓Parametric studies
  - ✓Time evolution



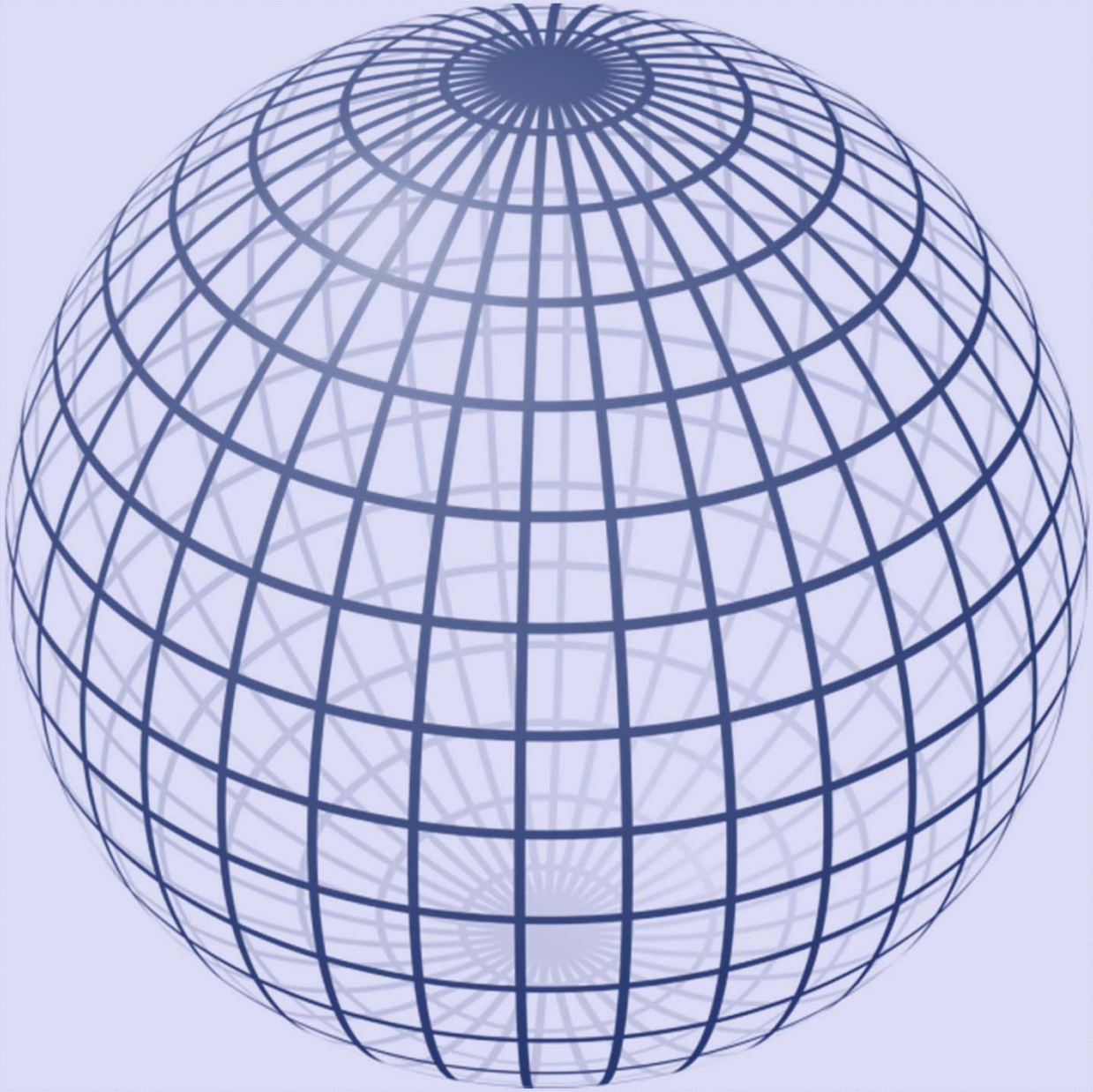
http://wwwmpa.mpa-garching.mpg.de/gadget/hydrosims/sim3d.png

Direction of the Field

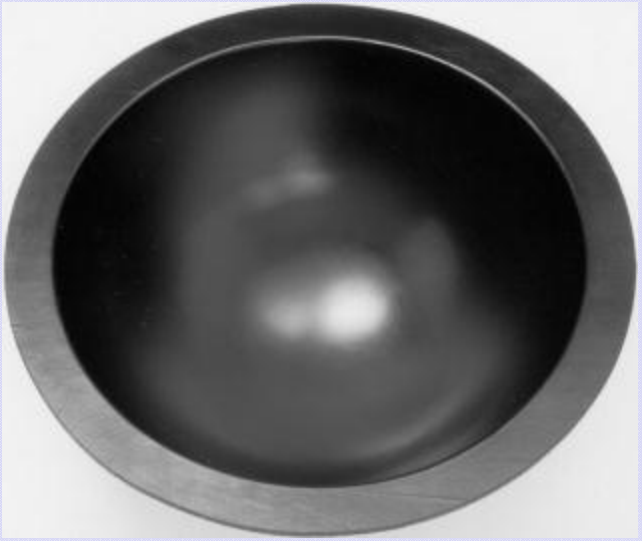
- Computer Modeling/Simulation: useful in three types of problems:
  - ✓Insoluble by traditional approaches,
  - ✓Hazardous to study in the laboratory,
  - ✓Time consuming or expensive to solve by traditional means.
- Some say : Classical approaches are not sufficient to understand the behaviour of real systems: New knowledge creation.
- ✓Others say: Models/simulations enable us only to examine our own "knowledge" from different points; no new knowledge is directly created.



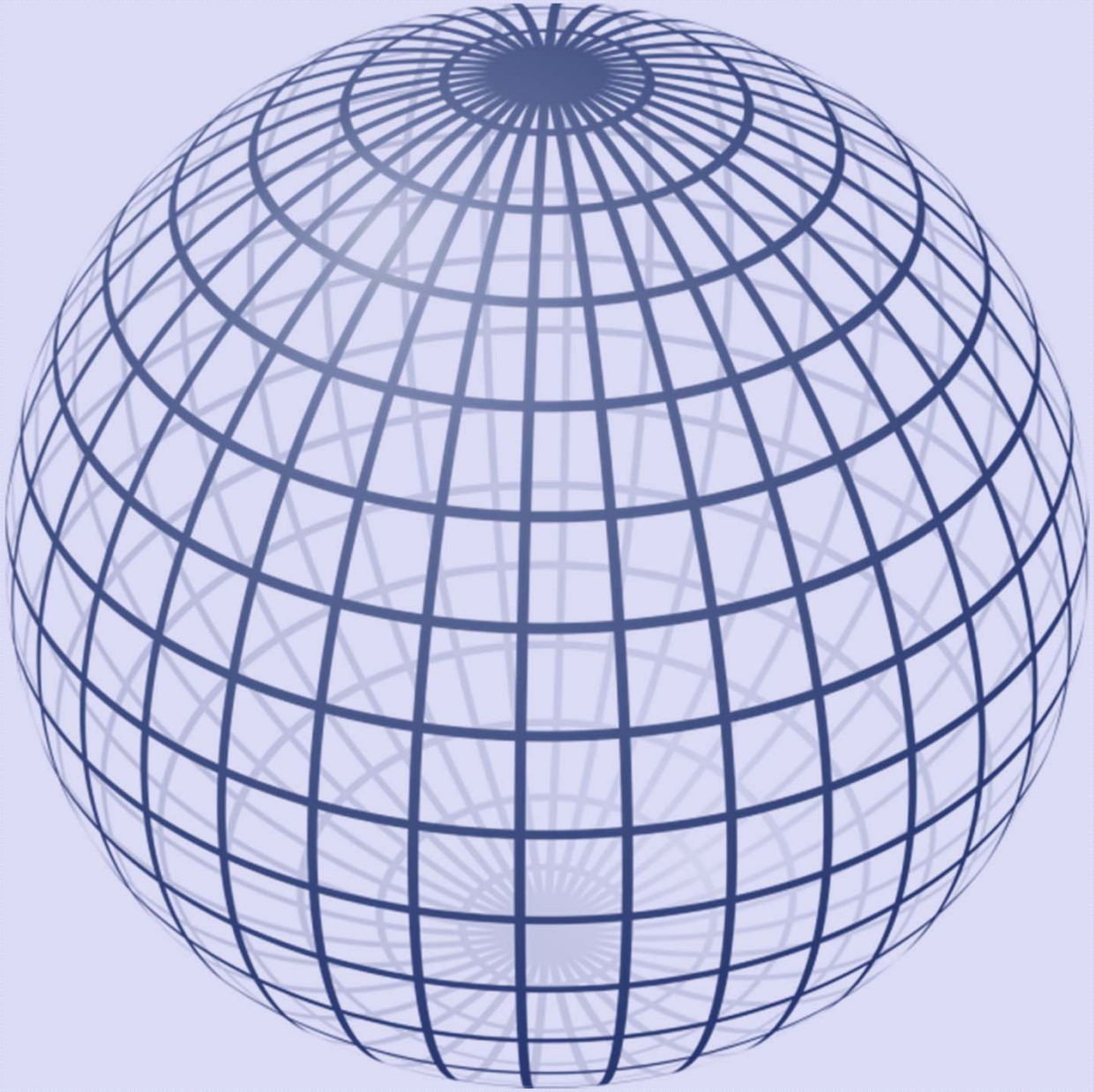
Observation:
Front view



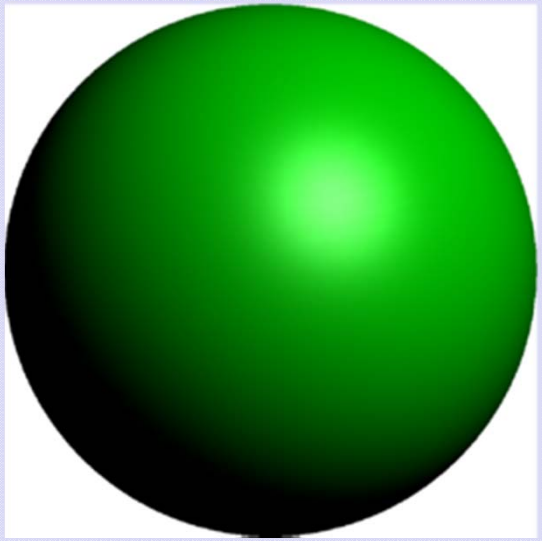
3-D Model

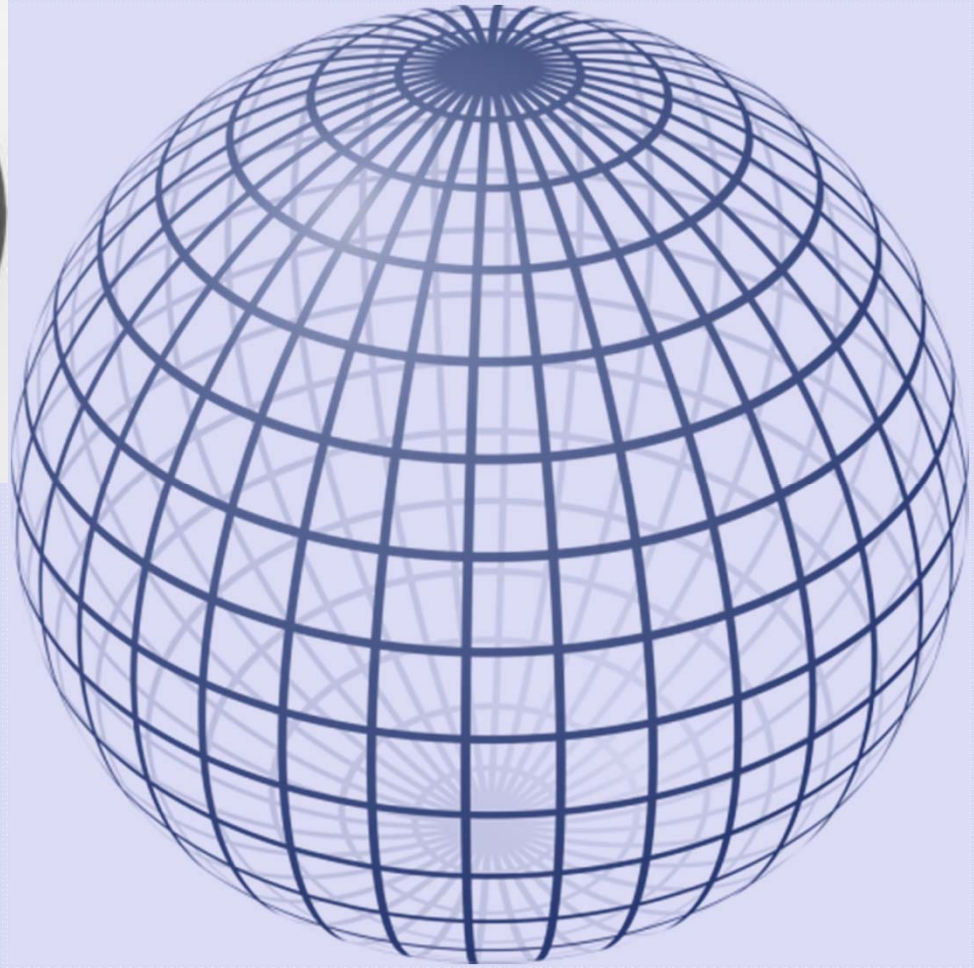


Observation:
Back view



3-D Model needing modification



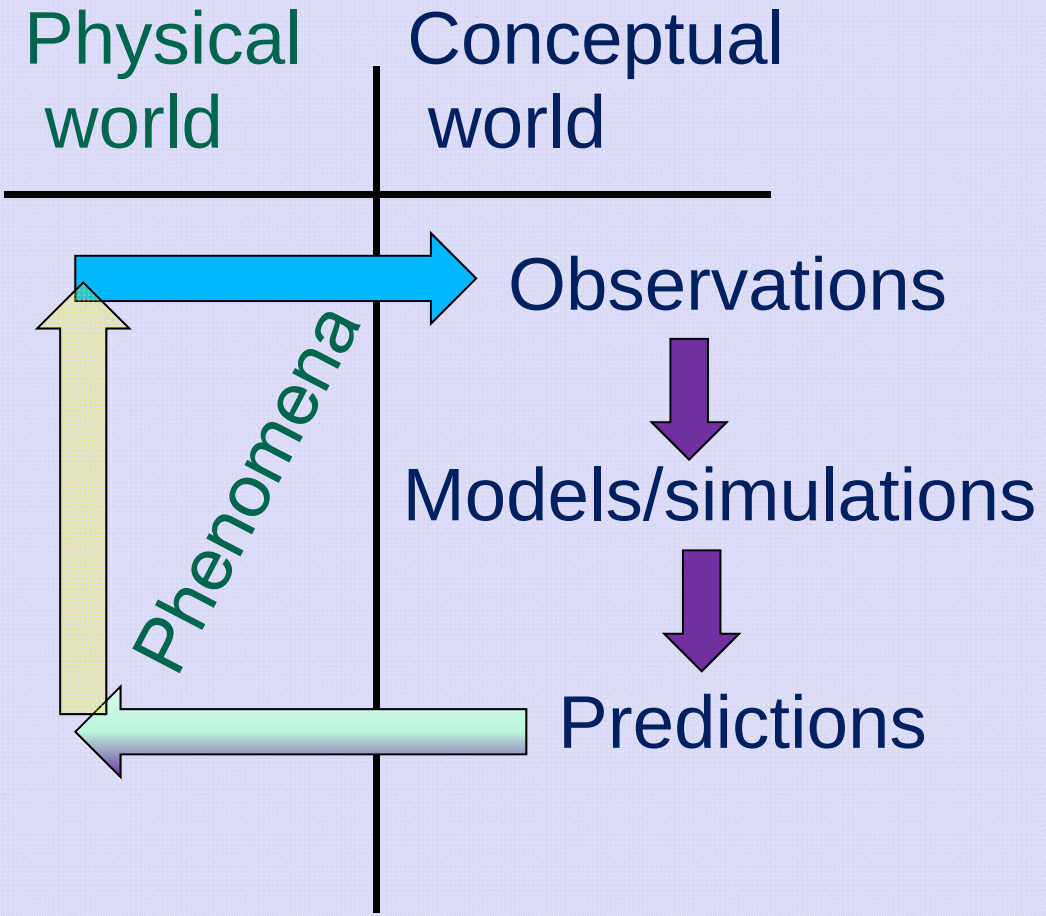


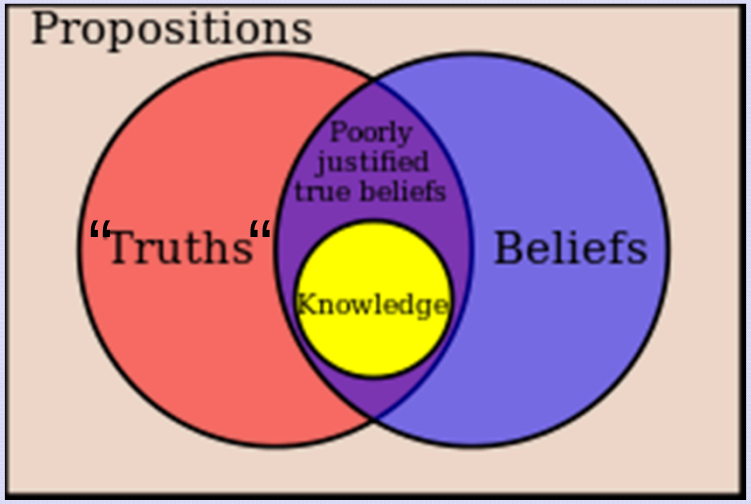
The basic dilemma in the process of validation: a mathematical analogue can be validated only in a given number of known situations. Perfect validation is not possible. ***Panjabi (1979)*** "

Scientific models fit the system similar to the way maps fit the world (Giere, 1999)

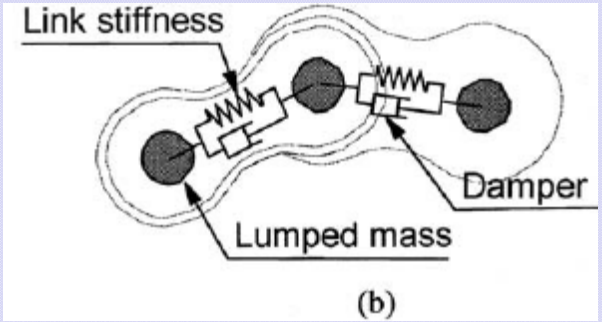
➢Conclusions from models are based on ' surrogative reasoning'.

Thus, information from models need a careful epistemological analysis.



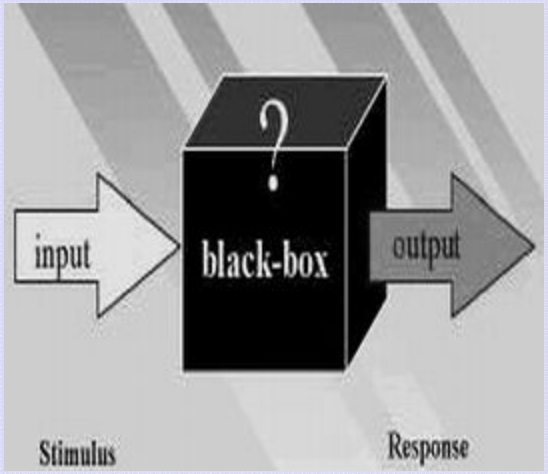


- **Learning with Models takes place:**
  - During the construction of the model.
  - During the manipulation of the model.



- **Problem of validation**

  Do the equations in the model represent the target system with sufficient accuracy?

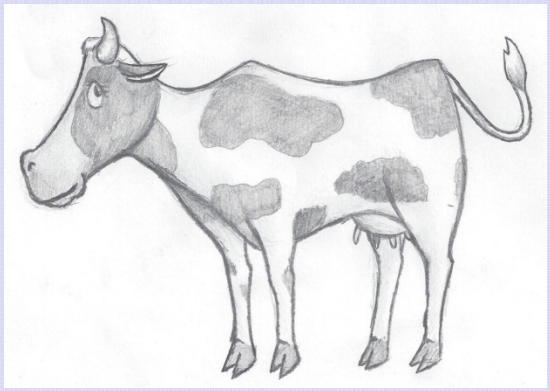


- **Problem of verification**

  Does the computer provide accurate enough solutions of these equations?

- Interpretation of results from models or simulations can be quite risky without fundamental understanding of the system.

- A properly constructed model can be used to check our understanding of the equations we use.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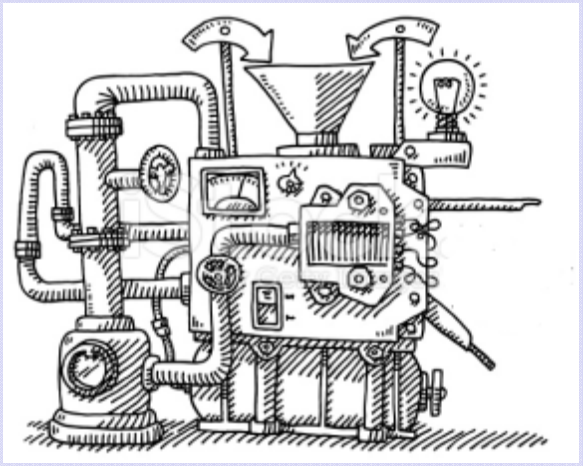
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A model should be used in the reverse direction as well!

- Comparison of the output of the inverted model enables us to see if we truly understand what is going on.

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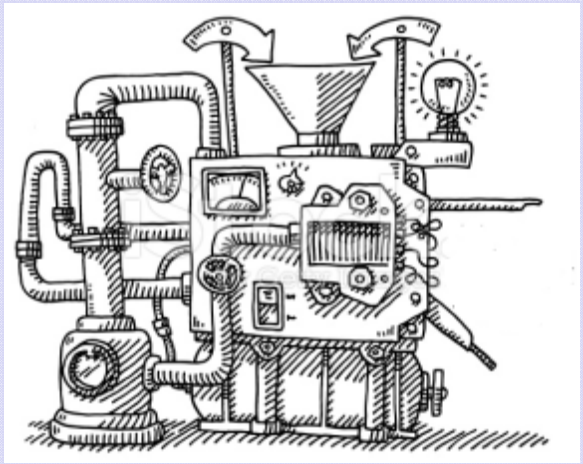

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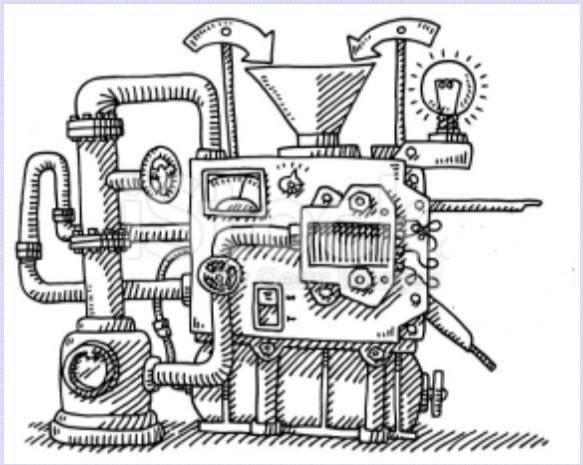

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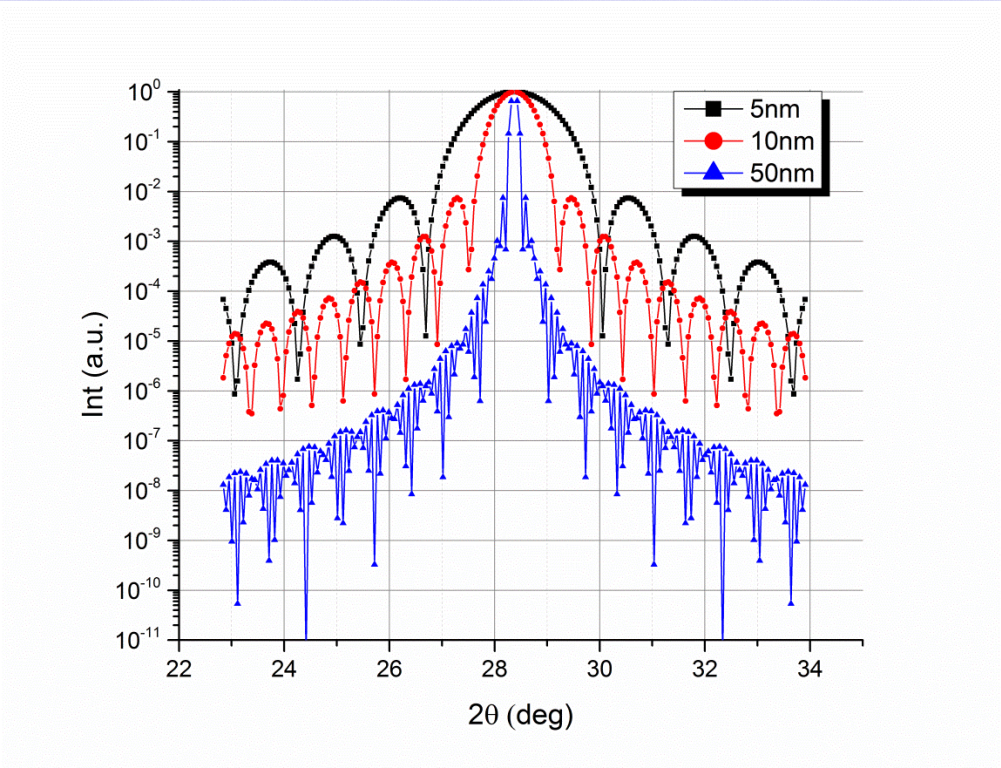
- A non-invertable model indicates a badly-posed inverse problem.

- Most models with too many fitting parameters are of this kind.

Examples from our work

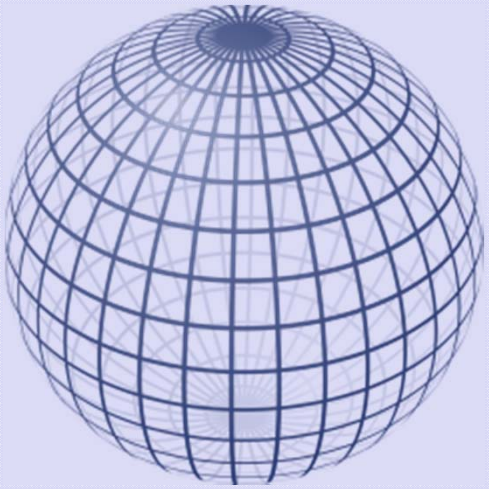
Please see:

- *Sampling statistics of diffraction from nanoparticle powder aggregates*, H. Öztürk, H. Yan, J. P. Hill and I. C. Noyan, . Appl. Cryst. (2014). 47, 1016-1025 doi:10.1107/S1600576714008528
- *Correlating sampling and intensity statistics in nanoparticle diffraction experiments*, H. Öztürk, H. Yan, J. P. Hill and I. C. Noyan, J. Appl. Cryst. (2015). 48, 1212-1227 doi:10.1107/S1600576715011747



Summary & Conclusions

- Mathematical modeling/simulation can be very useful in teaching and research.
- Students should be taught how to create models and, in the process, how to evaluate models.
- Black-box models with inadequate documentation should not be used in either research or teaching.
- In the end, we should not lose the "feel" for equations and numbers.



- Computers should be used as tools, not consulted as oracles.

- Nor should we overlook the role of serendipity in discovery.
  - **Age Hardening** (Wilm, Berlin, 1906)
  - **Stainless Steel** (Brearley, Sheffield, 1913)
  - **Superalloys** (1930-1960); Ni-Al-Ti system.
- *There is still a place for thought and experimentation in the scientific method.*

"The symbol is NOT the thing symbolized:
the word is NOT the thing;
the map is NOT the territory it stands for."

—S. I. Hayakawa, "Language in Thought and Action"

Dear Department of Metallurgical and Materials Engineering

Thanks for a wonderful education.

THANK YOU FOR YOUR ATTENTION