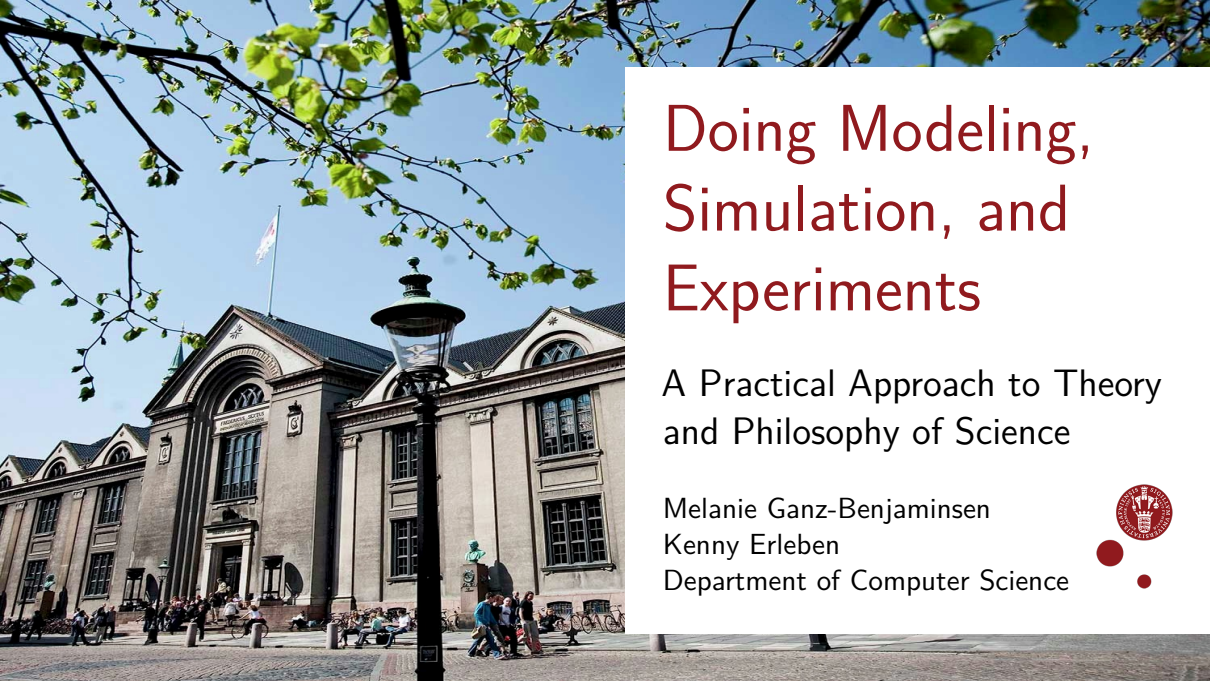

Doing Modeling, Simulation, and Experiments

A Practical Approach to Theory and Philosophy of Science

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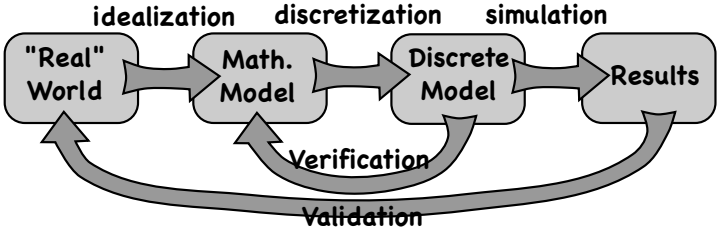
Philosophy?

Every researcher has his own story – this is my story

A Conceptual Data Flow Diagram



Idealization: Stating a mathematical model

Discretization: Converting into a discrete model/numerical method

Simulation: Computing simulation results

Verification: Agrees with the mathematical model (Are you computing solutions to the problem?)

Validation: Can be applied to real-world (Are you solving the right Problem?)

Different Approaches to Modeling

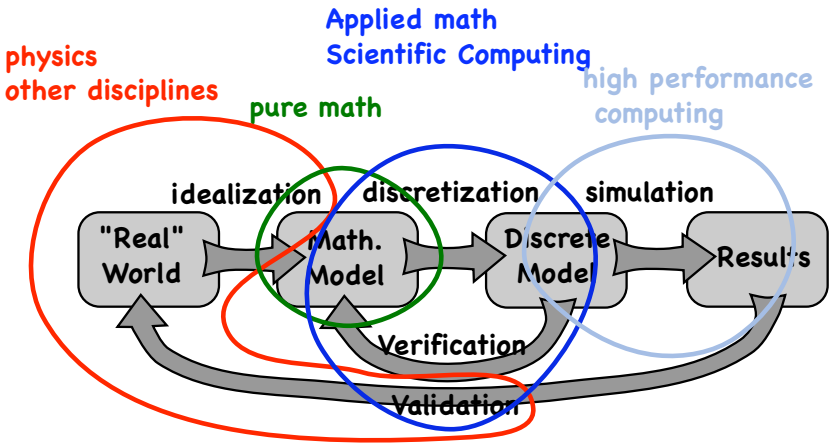
Two categories may be defined

Data-Driven Modeling: Starts by looking at data for example images of real-world objects and creates a model of the data.

Method Driven Modeling: Often uses laws of physics (math formulas) or similar to creating a model of a real-world problem.

One could argue they are duals of each other in the sense of whether data or math comes first.

Cross Disciplinary Effort



Many players... can you find yourself?

We need Experiments when Modeling

- Verification
- Validation

Question

What is an experiment?

Dictionary Answer

A test under controlled conditions that is made to demonstrate a known truth, examine the validity of a hypothesis, or determine the efficacy of something previously untried

(From The American Heritage® Science Dictionary)

Question

How do we conduct a good experiment?

The Hornbæk Advice

Before doing an experiment:

- Think about validity and reliability
- Design so as to rule out alternative hypotheses
- Consider treatments and measures

While doing an experiment:

- Minimize variability
- Minimize experimenter's influence

After doing an experiment:

- Do statistical analysis
- Discuss validity and sources of error

The Ingvor Advice

- What is the purpose of the experiment?
- Which and how many variables/parameters affect the experiment?
- Estimate if one has enough data for the experiment
- Estimate the time needed to conduct the experiment
- State the theoretically expected results of the experiment

The Erleben Advice

Start Backwards

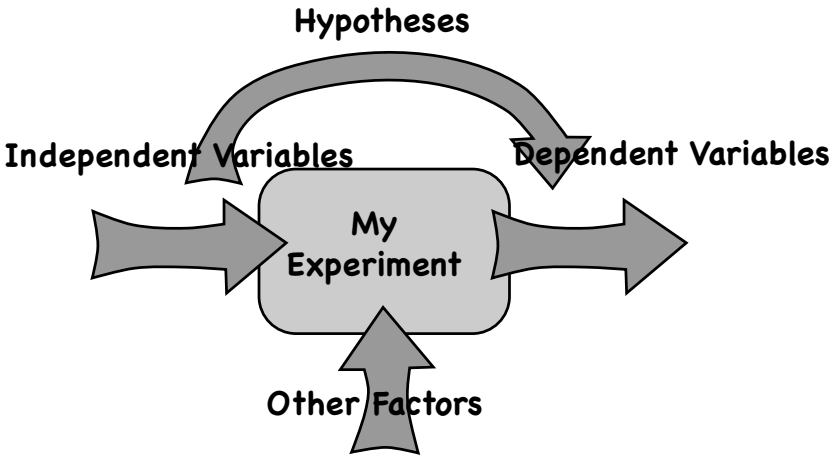
- Do experiment planning early
- Create “competing” solution before your own
- Get practicalities out of the way first

Some Semantics of Experiments

- Hypotheses
- Validity
- Reliability
- Variables

Now we will look at these words in little more detail

Schematic Overview



Question

What is a hypothesis?

Dictionary Answer

A tentative explanation for an observation, phenomenon, or scientific problem that can be tested by further investigation.

(From The American Heritage® Science Dictionary)

Formulating Hypotheses

Good hypotheses:

- Are developed early
- Define independent and dependent variables
- May be motivated by theory or literature
- Are concrete, specific, clear
- Can be shown wrong

Hypotheses help think about one's work

(From Kasper Hornbæk)

Validity

Internal Validity:

- Showing that the changes in the independent variable cause the observed values of the dependent variable
- Ruling out rival hypotheses

External Validity:

- Are findings repeatable?
- Do findings generalize across settings and populations?

Reliability

- Reliability is the consistency of a measuring instrument or among measurements
- Reliability concerns for instance agreement among observers, similar measures at other times

Variables

Two types

- Independent Variables/Parameters
- Dependent Variables/Parameters

Think of it as

$$y = f(x)$$

Practical Examples of Verification and Validation

What can we do?

Properties of a Mathematical Model

Mainly concerned with two questions

Existence of a solution?

and

The uniqueness of the solution?

Properties of a Discrete Model

- Robustness
- Efficiency
- Accuracy
- Convergence
- Scaleability
- Stability
- Sensitivity

Robustness

They should perform well on a wide variety of problems in their class, for all reasonable choices of the initial variables.

(From Nocedal and Wright)

Efficiency

They should not require too much computer time or storage

(From Nocedal and Wright)

Accuracy

They should be able to identify a solution with precision, without being overly sensitive to errors in the data or to the arithmetic rounding errors that occur when the algorithm is implemented on a computer.

(From Nocedal and Wright)

Scaling of Problem

In unconstrained optimization, a problem is said to be poorly scaled if the changes to x in a certain direction produce large variations in the value of f than do changes to x in another direction

(From Nocedal and Wright)

Scaleability

In general we talk about properties of an algorithm. In particular storage complexity and computational complexity etc.

(From Nocedal and Wright)

Stability

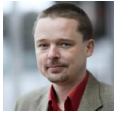
Stability is a property of the Algorithm. An algorithm is stable if it is guaranteed to produce accurate answers to all well-conditioned problems in its class, even when floating point arithmetic is used. ... A problem is said to be well-conditioned if its solution is not affected greatly by small perturbations of the data that define the problem.

(From Nocedal and Wright)

Sensitivity

Given a measure E to be minimized wrt. the parameters a, b, c, etc.. Assume a minimizer, $dE = 0$, next vary parameters a,b,c, etc. and estimate second-order moments. If they are large then E is very sensitive. Or add noise... in a controlled manner and see if things blow up!

(From Jon Sporring: Practical Scientific Paradigms...)



Convergence

Local Convergence: What happens if we are in a neighborhood close by to a solution to our problem?

Global Convergence: Can we find a solution?

Global Convergence

Warning: The term globally convergent refers to algorithms for which the property

$$\lim_{k \to \infty} \| \nabla f(x^k) \| = 0$$

is satisfied.

Question

How to show physical correctness?

Conservation Laws

From physics:

- Mass conservation
- Momentum conservation
- Energy conservation

Physical Plausible?

- Human perception?
- User tests?

(Talk to Kasper Hornbæk)

Compare Results

- Real-world experiments
- Results published by others
- Results created from other software

Any problems with these ideas?

Question

What is an error?

(Hint: Remember the data flow diagram)

Some Partial Answers

- Modeling error
- Discretization error
- Implementation error
- External error sources (the computer?)
- Yourself –- wrong insight of what is to be expected!

Last Question!

Is program testing an experiment?