Models & Simulations Conference 4 (Toronto, May, 7^{th}-9^{th} 2010)

Tools or Toys?

On specific Challenges for Modeling and the Epistemology of Models & Simulations in the Social Sciences

Stuttgart Research Center
for Simulation Technology
http://www.simtech.uni-stuttgart.de/

Eckhart Arnold

- General Epistemology of Models
- Example: Simulations in Chemistry
- Opinions on Social Simulations
- The Difference, the Social Sciences make
- What we can do about it
- References

Epistemology of Models
Example: CS in Chemistry
Models in Soc. Science
Differences of Soc. Sciences
Challenges and Responses

1. The Epistemology of Models

The Role of Models in Science

Epistemology of Models
Role of Models
Credibility of Models
Simulations and Models
Simulations and Experiments

Models are "Mediators" between Theory and Empirical Reality:

Theoretical Foundation

Models are derived from theories. They contain laws of nature from theories.

Semi-Autonomy

Models involve model building techniques not derived from background theories.

Target System

Models have target systems in the real world which they represent.

References: [MM99, Win03]

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Sources of Credibility of Models:

- Credible background theory and background knowledge
- Well approved modeling techniques
- Successful empirical tests

Rules of Credibility

- Successful empirical tests trump background theory and modeling techniques
- The smaller the credibility of one source, the greater the strain on the others

"Same old stew"

Simulations are models (w.r.t. validation)

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- Opacity?

Only the process of simulation is opaque not the algorithms.

- Computational process replaces deduction from axioms?

Models just as simulations are semi-autonomous.

- Temporal dynamics matter?

True, but introduces no new issues concerning the validation of simulation.

- Distinction between "in principle" and "in practice"?

What is possible "in practice" matters. But again, no difference to models.

References: [FR09, Hum04, Hum09]

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Simulations are not experiments

- Simulations only yield results that are implied by background theories and simulation assumptions
- No causal influence from the target system on the results
- *Experimenta crusis* not replacable by simulations
- Only some experiments ("analog computations") replacable

Therefore: Simulations – just like models or theories – belong to the theoretical side of science!

References: [Mä05, KL05, Win03, Mor09]

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Models in Soc. Science
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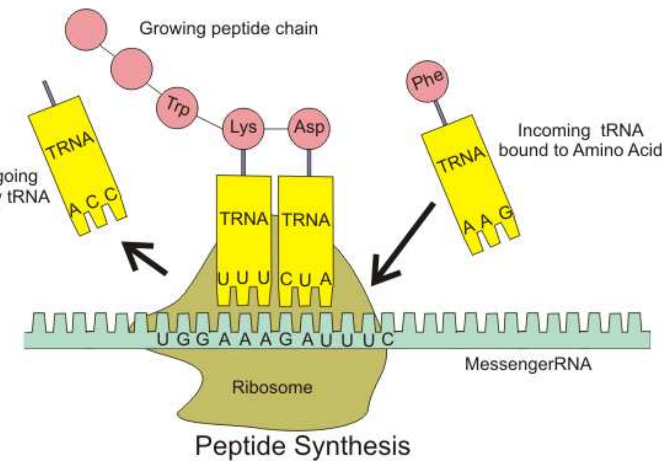
2. Example Case: Computer Simulations of Peptid Bond Formation in Chemistry

Acknowledgement: I'd like to thank Prof. Johannes Käster, Insitute of Physical Chemistry in Stuttgart, for explaining this type research to me!

Ribosomes: Protein Factories of Living Cells



The ribosome catalyzes the peptid bond formation between amino acids (image source: wikipedia)

Current research questions:

- How does the ribosome catalyze? Spatial arrangement or electrostatic influence?
- How does the reaction take place? (Different mechanisms imaginable)

Problem: Experiments can only determine the reaction energies!

References: [KS10, wik10]

Example: CS in Chemistry
Ribosomes
Simulations of the Ribosme
Epistemological Reflection

Simultions of the ribosome

Approach

- QM/MM-simulations of the ribosome of the *thermus thermophilus* bacteria
- Multiple techniques for approximation and optimization to lower computing time

Results

- Electrostatic influence rather than spatial arrangement of molecules essential for catalysing the reation
- Two different reaction mechanisms possible, possibly both competing in nature

Confirmation?

- Activation energy found in simulations matches experimentally determined values
- Mismatch in one particular scenario, calling for explanation and giving rise to new research questions

References: [KS10]

Epistemological Reflections

- All three sources of credibility involved
- Powerful physical background theories exist
- Comprehensive prior knowledge about the ribosme
- Empirical data to test part of the simulation results
- Reliability of approximations and quality of experimental data may raise further questions

(Expert knowledge required to assess these)

References: [KS10]

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3. The role of models & simulations in the social sciences

Brief overview of some recent accounts

Models & Simulations in the Social Sciences

Some striking, yet frequent features:

- Highly stylized and idealized
- Reliance on counterfactual or unrealistic assumptions
- Little or no empirical testing
- Few generalizable results
- Unclear epistemological role

"authors typically say very little about how their models relate to the real world" [Sug09, p.25]

References: [Sug09, Car09, Arn08, Sha05, GS94]

Models in Soc. Science
Striking Features
Diversity of Opinions
No Easy Solutions

Accounts of Models in the Social Sciences

1. Predictive devices
   [Fri53] But: Poor prediction qualitiy [Bet06] undermines this justification
2. Quasi-Experiments
   [Mä05] But: Epistemologically dangerous analogy
3. Isolating devices
   [Mä09, Car09] But: Analogy limited if not misleading [KL09]
4. Credible counterfactual worlds
   [Sug00, Sug09] But: Who determines the credibility?
5. Incredible worlds
   [KL09] But: Strong robustness requirement
6. Partial explanations
   [Ayd07] Good for a research design, but may not fit all modeling types
7. Tools for conceptual exploration
   Always possible fallback, but greater potential of modeling may be overlooked

No easy Solution:

Many diverse opinions, but no winner in sight

- Some of the accounts contradict each other sharply
- Most of the presented accounts relate to the same examples (e.g. Schellings neighborhood segregation model), so the incompatibility is serious
- Most of these accounts have some good reason on their side
- There is no obviously "better than all the others" account, although the "partial explanation" account seems a very strong contender.

Models in Soc. Science
Striking Features
Diversity of Opinions
No Easy Solution

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4. Differences between the Social- and the Natural Sciences that are relevant for Modeling

Differences of Soc. Sciences
Overview
No Universal Theories
Pluralism of Paradigms
Muliple Causality
Pluralism of Styles
Difficulties of Measurement

Specific Features of the Social Sciences

Obstacles for Modeling?

- Lack of well confirmed background theories
- Pluralism of paradigms as a normal state
- Multiple and varying causes for the same effect
- Pluralism of scientific styles
- Difficulties of measurement and lack of quantitative data

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Lack of universal Background Theories

No empirically well confirmed background theories in the social sciences that fully cover the phenomena in their domain

(as for example Newtonian mechanics in physics).

Epistemological consequences:

- Theoretical validation insufficient, empirical validation needed
- Unknown unknowns more abundant

Unknown unknowns cannot be excluded on the grounds that they fall outside of what some theory allows. (In contrast, in Chemistry we could probably say: "Nothing can happen that quantum mechanics does not allow.")

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Pluralism of Paradigms

Typical for the social sciences:
Pluralism of paradigms and multitude of competing theories

Example: In their book on the cuban misile crisis, Graham Allison and Philip Zelikow present three different paradigms, each of which encompasses a host of different theories and approaches, partly overlapping, partly contradicting and partly complementing each other [AZ99].

Epistemological consequences:

- **Phenomenological models better than theoretical models**

  For, theoretical models are more liable to merely reflect the presuppositions of the preferred paradigm.

- **Alternatives must be considered**

  The best way to avoid falling prey to the sugestiveness of one particular paradigm is consider things from the viewpoint of another paradigm.

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Multiple and Varying Causes of the same Effect

Many important phenomena in the social sciences are characterized by the fact that they may be caused in many different ways (e.g. outbreak of war).

Epistemological consequences:

- A demonstrated "theoretical possibility" is just a single piece in the puzzle
- Parsimony: a vice, not a virtue
- Other "possible explanations" to be checked as well

Other possible explanations that cannot be rendered in a mathematical model should not silently be ignored.

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Pluralism of Scientific Styles

Multitude of different scientific styles in the social sciences, e.g. thick narratives, stylized verbal descriptions, mathematical descriptions or hermeneutical methods.

Epistemological consequences:

- **Not only "models as mediators"**

The "last mile" between model and the raw empirical material is typically some sort of narrative description.

- **Challenge of integrating models with other methods**

The task of formalizing a verbal account is often highly non-trivial: Does the model really capture the essential aspects of the problem at hand? Does the formalized form still represent the verbal form? Etc.

- **Are models a reasonable option at all?**

Should be evaluated before constructing a model.

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Difficulties of measurement

In the social sciences, many phenomena are notoriously difficult to isolate, experimentation is often not possible and many factors cannot be measured precisely.

Epistemological consequences:

- Greater strain placed on the robustness of models
- Simple models often the best choice

Increase a model's complexity only if this is rewarded by greater explanatory power as testified by comparison with measured data.

- Where measurement is not possible, modeling is not worthwhile

Models may give a false sense of understanding and precision where we really know nothing.

References: [Sha05, GS94, Hum04, Arn08]

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5. Challenges and Responses

What modellers can do about it
and what philosophers of science should be aware of

Lessons for Modelers

Lessons for *problem orientated research*:

- Keep your options open: Evaluate other methods as well
- Choose wisely: If models do not work for your problem, try solutions without models.

Lessons for *method orientated research*:

- Chose the right problems for your method

i.e. problems where models work and their success can be tested.

- Keep in mind that your model needs to be validated empirically

Do not use unmeasurable parameters, mind the limits of measurement accuracy already at design stage.

- Validate your model, take failures seriously

A model that fails validation is wrong. A model that cannot be validated is unscientific.

References: [Sha05, GS94]

Lessons for Philosophers

Where modeling in the social sciences differs:

- Models “mediate” differently in the social sciences

On the theory side, there are only vage or non-unversal theories. On the empirical side models may need to link to narratives.

- Simulation-experiment analogy harder to justify

In natural sciences this analogy works, because powerful background theories and comprehensive background knowledge allow conducting “computer experiments”.

- Because of the lack of powerful background theories, empirical validation becomes even more important

- Philosophers should refrain from rationalising bad practices

If modelers themselves do not know, how their models relate to reality, then the most salient explanation is that their models are inappropriate.

Challenges and Responses
Lessons for Modelers
Lessons for Philosophers

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Models in Soc. Science
Differences of Soc. Sciences
Challenges and Responses

Thank your very much for your attention :)

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