Philosophical Issues of Computer Science
Computer Simulations and Experiments
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Explorative experiments as forms of directly action-guiding experimentation

- Devoted to testing technical artifacts
- Focused on iteratively refining the intervention (not testing a general theory but probing the possibilities and limits of the intervention)
- No sharp distinction between designers and experimenters (often practitioners becoming experimenters)
- Control of the experimental factors not fully managed from the beginning, but in part carried out after the insertion of artifacts into their environment
Computing and experiments

- The nature and role of experiments in computer science (CS as science)
- Computer simulations as tools for other scientific disciplines (CS as infra-science)

- Computer simulations as experiments (also explorative experiments)
Simulation is the reproduction of the behavior of a system using another system, providing a dynamic representation of a portion of reality (Hartmann 1996)

Example: scale model of a bridge built to test the resistance of some materials to atmospheric agents

- Model not enough for the purpose
- Need of putting it in a controlled physical environment
- Model executed in the reality by means of the action performed by the environment
Model + execution

- Simulation: model + execution
  - **Model** as a *representation* of the aspects relevant to a specific purpose
  - **Execution** of the model as the process *performed* by an agent (natural environment, human being, computer)

- Simulation can be seen as an *executable representation*
Computer simulations

- Simulation is based on a computational model and executed by a computer
  - Computational model: formal mechanism able to manipulate strings of symbols (to compute functions)
- Computer simulation is the process resulting from the execution of a computational model representing the behavior of a system whose state changes in time
  - Not every execution of a computational model is a computer simulation!
Classification of simulations: a tentative proposal

- It is possible according to two different dimensions
  - Type of model
  - Agent performing the execution

- Computational model (formal mechanism able to compute functions): execution performed by a computational machine (computer)

- Mathematical model (e.g. system of equations): execution performed both by a computer and a human being

- Physical model (representation of a selected part of the world): execution performed by the nature itself
- Computational science introduces new issues into the philosophy of science because uses methods that push humans away from the center of the epistemological enterprise (Humphreys 2004)
- Anthropocentric predicament: how we humans can understand and evaluate computationally based scientific methods transcending our abilities
There exists a variety of positions

- Simulations ‘just’ as techniques for conducting experiments on digital computers (Naylor 1966)
- Simulations as intermediate tools between theories and empirical methods (Rohrlich 1991)
- Simulations as substitutes for experiments impossible to make in reality (Hartmann 1996)
- Simulations as novel experimental tools (Humphreys 2004)
- Simulations as special kinds of experiments (Simpson 2006)

The more radical one is the “identity thesis”

- ‘Computer simulation studies are literally instances of experiments’
Simulations used as experiments

- It is possible in case of coincidence between purposes of simulations and experiments (Peschard 2012)
  - Discovering new explanatory hypotheses, confirming or refusing theories, choosing among competing hypotheses, ...

- But not necessary
  - Simulation with no experimental purposes (e.g. simulation of a protein folding process for didactical purposes)
- **Similarity** between techniques of experimentation and techniques of simulation (Winsberg 2010)
  - Involvement of *data analysis*
  - Constant concern with *uncertainty* and error

- **Experiments** and **simulations** (used for experimental purposes) as forms of controlled experience
  - Ability and necessity of *controlling* the features under investigation
  - Choice and control of the experimental factors (artificial setting)
Practical reasons

- (Computer) simulations used as experiments
  - To make several accelerated experiments exactly repeated and with a high precision degree non always possible in empirical cases
  - To perform experiments difficult to make in reality being free from many of the practical limitations of real experiments
  - To carried out experiments impossible to make in reality, such as studying parts of reality not physically accessible
From techniques to derive numerical solutions to systems of differential equations with non analytical solutions (typical of physics)

“Any computer-implemented method for exploring the properties of mathematical models where analytic methods are unavailable” (Humphreys 2004)

To explorations to develop new hypotheses, models, and hints to be further verified and to construct models of phenomena in the absence of theoretical base (typical in some areas of biology)

- Theoretical model behind simulation under construction and shaped by simulation results
Simulations without theories

- How simulation models can be constructed without the recourse to a theory providing the structure and dynamics of the investigated phenomenon?
- Non-theoretical starting points
  - *Modeling from above* (Fox Keller 2002)
  - *Modeling from the ground up* (MacLeod and Nersessian 2013)
Integrative computational system biology
- Application of computer technology to what formerly considered inaccessible complexity (from ecological systems to genes) to generate representations of the dynamics of these networks
- Theory of biological systems emerging from model building and simulations (and not theory producing simulations)

Bottom-up strand of system biology
- Simulations built from the “ground up”
- Principles from molecular biology, experimental results, literature surveys, canonical models, and computational algorithms pieced together in a nest-like fashion
An ethnographic approach

- **Modeling from scratch** (not from a theoretical starting point)
  - Empirical information from different sources pieced together into a representation using assumptions and simplifications and mathematical and computational techniques

- **Iterative and incremental** model building process
  - Preliminary simulations to understand systems and adapt representations
  - Refinements and revisions

- **Exploratory process**
  - *Functional role* of simulations for learning how to assemble information and construct computational models without starting from a theoretical basis
A different kind of modeling

- Simulations are directed to augmenting the exploration opportunities at two levels
  - Possibility for users to test reactivity and adaptability of the model in progress
  - Shaping the theoretical model under construction on the basis of simulation results
Exploring knowledge **without** the grounding in real physical processes (neither in well-founded theories nor in experimental data)

- Simulation results suggesting new regularities not extractable from the model assumptions otherwise

Getting some **hints** for new knowledge **to be further investigated**

- Explorative in the sense of not giving the assurance of the correctness of a conjecture, even if helping to build it up

Spatial (access to inaccessible parts of reality), temporal (acceleration of real temporal scale), and **conceptual** expansion of the realm of investigation (**“playing in the wild”**)

Computer simulations as explorative experiments
Validating results

- Usually two approaches are adopted
- Simulation models are strongly grounded in well-founded theories
  - Simulation of physical phenomena already modeled by equations
- Simulation results are compared against experimental data
  - Simulation of artificial phenomena and processes comparable to real phenomena and processes
Credibility at issue

- What happens when simulations as explorative experiments are used in substitution of real experiments?
- How to validate simulation results in absence of theoretical ancestors or well grounded data?
- What reasons to believe in simulations and their experimental power even in these cases?
Reliability

- From verification to reliability
- **Reliability without truth** (Winsberg 2006)
  - Not only less strong, but implying a shift in the perspective
  - No yes or no answer, but different degrees
- Different strategies for assessing reliability
No strategy

- No need of any strategy
- Use of simulation is narrow
  - Simulations adopted just for pictorial purposes with didactical, explicative, or clarification means
    - Simulations of the 3D protein folding or the DNA helix
  - Simulation is strongly rooted in previous knowledge
    - Exploration/experimental purposes reduced to a minimum
Minimal strategy

- *In virtuo* simulation, *in vitro* validation
- Simulation tools are exploited theoretically to explore new scientific knowledge
  - Simulation as a ‘trial theory’ (Fox Keller 2003)
- Simulation results are validated experimentally in a continuous manner
 Variety of situations in the simulation framework
  - Presence of incomplete empirical data
  - Weakness of theoretical framework
  - Difficulty in making experiments

 Not a single strategy is needed, but a pool of strategies providing reasonable belief in simulation results
Inference from success to reliability

- Sources of credibility for simulations
  - Prior success of the model building techniques adopted
  - Production of outcomes fitting well with previously accepted data, observations, and intuitions
  - Capability of making successful predictions
  - Capability of producing practical accomplishments
  - ...
Pluralism and fallibilism

- No general rule exists on how to combine and use these strategies
  - Local solutions to be founded in each different situations
  - Not easy to understand how to locally apply them
- There are good reasons to assess simulations reliability, but in a fallibilist perspective (Hacking 1983)
  - No guarantee of the correctness of the results: even when strategies are applied, simulation results can be shown later to be incorrect
Computer simulations as controlled experiments

- Set of observations and actions, performed in a controlled context, to test a given hypothesis
- Simulations implement a way of choosing and controlling experimental factors
  - Anticipatory tools in substitution of real experiments (*learning-by-anticipation*)

Computer simulations as explorative experiments

- Investigation of a real of different possibilities to get some hints for new knowledge to be further investigated
- Simulation results shape the theoretical model under construction
  - Explorative tools to learn things that cannot be learned by anticipation (*learning-by-experimentation*)
References

- Radder H. (ed.) The Philosophy of Scientific Experimentation, Pittsburgh University Press