METHODEN 1

Valerie Feldmann, Katrin Mühlfeld (eds.)

VIRTUAL WORLDS OF PRECISION

Computer-based Simulations in the Sciences and Social Sciences

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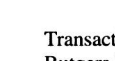

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Foreword

In recent years, the use of computer simulations to gain a deeper understanding of complex dynamic systems in all scientific disciplines has become widely accepted. Computational science is becoming established as a third way of understanding reality besides the classical approaches of theoretical reasoning and experimentation. Modelling and simulation are two of the most successful tools developed in this field because they are universal and widely applicable. Basically the same methodology is applied in the natural sciences, in the engineering sciences and even in the social sciences although the aims and preconditions may be very different.

In the past, the technical details of simulations always required mathematical skills, programming and large computer resources. Due to the still growing computational power of digital computers and the commercial availability of powerful and flexible simulation tools, several technical limitations that hindered the application of simulation methods in the past no longer exist today. Thus, simulation is becoming an "everyone's methodology" which is increasingly used even by non-specialists.

As a consequence of these developments, the enthusiasm for these new possibilities nowadays produces strange visions of virtual realities, virtual laboratories, virtual cells, virtual engineering, virtual worlds etc. This is where the dark side of power lies... Being more and more virtual, we are replacing reality with an artificial world until finally the original intention to gain more insight into reality is perverted. The only things that can be learned in a virtual world are the laws of this world which have been designed by their creator. Piquantly, in most cases this is the same person who implemented the program.

The only way to avoid the dangers of simulation and to keep a critical distance to our own virtual creations is to stay in contact with reality and to continuously discuss the methodological foundations of modelling and simulation. Fortunately, computational science is an interdisciplinary research field per se and, thus, it should be easy to communicate over the fence of our own garden. Doing this, we will see that other simulationists have similar problems although the aims of simulation projects are quite different. In particular, the question of model validity is posed in quite different ways that depend on the available data and knowledge.

For example, a natural scientist can usually control the experimental conditions in a much stronger way than a social scientist. To discuss the problems in different disciplines will certainly help to reflect on our own problems and to gain a critical distance to our technical work which often enough is just fiddling around with computational details.

This was also the intention of a research colloquium organised by the German National Academic Foundation at Trinity College at the University of Oxford in January 2003. The participants, having their scientific origins in very different scientific disciplines, presented their research on modelling and simulation with a strong focus on the relation between reality and simulation. The contributions range from astronomy and cosmology over theoretical chemistry, biology and medicine to the economic sciences. They impressively demonstrate the interdisciplinary discussion culture that is actively operated by the scholarship holders of the German National Academic Foundation. As long as this academic culture of interdisciplinary communication is continuing, we need not be afraid of becoming trapped in some virtual world.

Prof. Dr. Wolfgang Wiechert
Department of Simulation
Institute of System Engineering
University of Siegen

Preface

"**simulate**, *verb transitive.* Feign, pretend to have or feel, put on; pretend to be, act like, resemble, wear the guise of, mimic,....So **simulation**, *noun.*"

This definition in the *Concise Oxford Dictionary* covers well some general elements of the original use of the word. At the same time, it fails to capture an important connotation of the word as it is often used in academia: simulation as a scientific method nowadays often implies computer-based simulation. In fact, as *Byron Morgan* emphasizes in his seminal book "Elements of Simulation", simulation as it is applied and taught today would not have been possible without the computer revolution of the 20^{th} century.

Since its emergence as an important research tool in the past century, an enthusiastic and ongoing exploration of useful applications of simulations to various fields of research could be observed. However, sometimes this development overshadows some fundamental questions. Are computer-based simulations in the natural and social sciences really *the* new way to reach innovative research results? Or is the precision of computer simulation-based results all too often misleading and tempting such that the still present modeling restrictions are overlooked? The answer is important scientifically as well as in its economic, political and social dimensions. Simulations have reached new levels of precision with the acceleration of progress in computing and processing power. The amounts of data that can be processed and analyzed allow new methodological advances and inspire researchers across disciplines to tackle new research questions. The objectives of this edited volume therefore are

- to identify recent areas of research in which computer-based simulations allow for results and conclusions that would have not been possible without simulations,
- to evaluate the opportunities and the limits of computer-based simulations, and to foster trans-disciplinary scientific work that explores the potentials of e.g. methods of theoretical physics for areas of economic research.

The significance of advanced simulation methods is a well-accepted fact in most areas of sciences and is being recognized as an emerging methodological paradigm

shift in other disciplines such as the social sciences. This edited volume is an essential compilation of areas in which this has been recognized already. However, we strongly believe that there is a lot more potential in the use of computer-based simulations for future research. Against this background, we are very pleased to have won an outstanding group of authors who each present their particular perspective on the applicability of computer simulation for their respective research area As a result, this edited volume covers a broad spectrum of questions associated with computer-based simulations. The variety reaches from areas of mathematics, physics, biology, and chemistry to economics and astronomy.

This edited volume comprises three distinct sections that analyse simulations in micro-, meso- and macro-structures. It explores simulations as a tool to receive information on experimentally inaccessible microorganic systems (von Lieres); as an approximation to unresolvable mathematical equations in valence ionization spectra of small molecules (Müller); in terms of optimisation of medical images of the human anatomy (Uhlemann); as an alternative to costly field trials in agricultural host-parasite systems (Grenz); as a tool to assess collective outcomes in economic systems resulting from the interaction of individual agents' behavior (Feldmann/Muehlfeld); as a means to estimate distributions in financial markets (Popovici); as solution to theoretical questions in general relativity where both analysis and experimentation fail (Löffler); and as a means for extrapolations concerning astronomical phenomena (Pauli).

The contributions are based on the presentations and discussions of the papers at the PhD research colloquium "Virtual Worlds of Precision" that has been held at the University of Oxford, Great Britain, from January 10–12, 2003.

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Berlin, London, November 2003

Valerie Feldmann
Katrin Muehlfeld

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List of Contributors

Following are the primary affiliations of the workshop participants including editors and chapter authors at the time of the workshop as well as at the time of publication.

Participants including editors and authors:

Bruce Edmonds
Centre for Policy Modelling
Manchester Metropolitan University
Manchester, UK

Valerie Feldmann,
formerly:
Economics and
Mass Communication
Free University Berlin
Berlin, Germany;
currently:
Affiliated Researcher at
Columbia Institute
for Tele-Information
Columbia Business School
Columbia University
New York, New York, USA

Tobias Galla
Department of Physics
Theoretical Physics Sub-Department
University of Oxford
Oxford, UK

Jan H. Grenz
Plant Production and Agroecology
in the Tropics and Subtropics
University of Hohenheim
Stuttgart, Germany

Sven Florian Kerstan
Department of Mathematics
King's College London
London, UK

Eric von Lieres und Wilkau,
formerly:
Institute of System Engineering
Department of Engineering
University of Siegen
Siegen, Germany;
currently:
Institute of Biotechnology
Research Centre Jülich
Jülich, Germany

Frank Loeffler
Max Planck Institute
for Gravitational Physics
(Albert Einstein Institute)
Golm, Germany

Katrin Muehlfeld
formerly:
Institute of Business-to-
Business Marketing
Westfälische Wilhelms-
University Münster
Münster, Germany;
currently:
Interdisciplinary Institute
of Management
London School of Economics
and Political Science
London, UK

Imke B. Müller
Institute of Physical Chemistry
Ruprecht-Karls-University
of Heidelberg
Heidelberg, Germany

Eva-Maria Pauli
Dr. Remeis Sternwarte
Astronomical Institute of the
University of Erlangen-Nürnberg
Nürnberg, Germany

Stefan Alex Popovici
Institute for
Applied Mathematics
University of Bonn,
Bonn, Germany

Falk Uhlemann
formerly:
Institute of Biomedical Engineering
Dresden University of Technology,
Dresden, Germany;
currently:
Institute of Artificial Intelligence –
Image Processing
and Recognition Group
Dresden University of Technology
Dresden, Germany

Introduction