COSY Workshop

Mathematical Modeling of Complex Systems - Lund, Sweden, September 5-7, 1996

Åström, Karl Johan; Schaufelberger, Walter; Mattsson, Sven Erik; Eborn, Jonas

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COSY Workshop

Mathematical Modeling of Complex Systems
Lund, Sweden, September 5-7, 1996

Karl J. Åström
Walter Schaufelberger
Sven Erik Mattsson
Jonas Eborn

Department of Automatic Control
Lund Institute of Technology
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Department of Automatic Control
Lund Institute of Technology
Box 118
S-221 00 Lund Sweden

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Author(s)
Karl J. Åström, Walter Schaufelberger, Sven Erik Mattsson, Jonas Eborn

Supervisor

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COSY Workshop, Mathematical Modeling of Complex Systems

Abstract

As a part of the European Science Foundation scientific program Control of Complex Systems a workshop on Mathematical Modeling of Complex Systems was held in Lund, September 5–7, 1996. This is a report documenting the purpose, presentations and conclusions of the COSY Workshop.

Modeling is an important aspect of complex systems. Models can result in drastic cost savings by reducing the need for experiments and are also useful for understanding the behavior of complex systems. European researchers have made substantial contributions to modeling, but the research community is fragmented. The COSY workshop brought together a number of European researchers involved in modeling and sought to find a common ground to stand on for a unification of the research efforts spent on modeling of the dynamic properties of complex systems.

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Contents

1. Introduction

The workshop on Mathematical Modeling of Complex Systems, which was held in Lund, Sweden, September 5–7, 1996 is part of the European Science Foundation scientific program Control of Complex Systems (COSY). This program has four research themes:

1. Control of Nonlinear and Uncertain Systems
2. Fault-tolerant Control Systems
3. Learning Control Systems
4. Integration of Complex Control Systems

The workshop is part of research theme 4 but it also has consequences for the other themes. Modeling is an important aspect of complex systems. The availability of models is a necessity for dealing with complex systems. Models can result in drastic cost savings because the number of experiments can be reduced significantly. Consequences of different strategies can be explored using the models and verified by a few experiments. Simulation of models is also useful for understanding the behavior of complex systems and for generating hypotheses for the development of theory. To be more specific the workshop was focused on modeling of the dynamic properties of complex systems.

European researchers have made substantial contributions to modeling. The research community is however fragmented. Modeling is a key part of control engineering and papers on modeling appear in the regular control conferences such as the IFAC World Congress, the European Control Conference, the American Control Conference and the Asian Control Conference. There are also results on modeling of complex systems in the special conferences organized by the large engineering societies, IEEE, ASME, AIAA and AIChE. There are also special conferences organized by IFAC and IEEE on Computer Aided Control System Design where a few sessions are devoted to modeling. Traditionally modeling has often been integrated with simulation. This is manifested in the simulation conferences organized by SCS (Society for Computer Simulation), IMACS (International Association for Mathematics and Computers in Simulation) and EUROSIM (Federation of the European Simulation Societies). In 1994 IMACS organized the 1. MATHMOD symposium which is devoted to mathematical modeling in Vienna, Austria. The next symposium will be held February 8–11, 1997 also in Vienna.

Although modeling is an important and time consuming activity that cuts across all engineering disciplines there are surprisingly few tools available. The available tools are also specialized to certain disciplines. This is a great difficulty when dealing with large systems that are composed of heterogeneous parts. In the workshop we had been able to gather 23 participants from 10 countries in Europe, see Appendix A. The age distribution of the participants was quite even, see the survey in Section 4.

The meeting covered a large part of the field, from theory to applications, from physical modeling to numerical mathematics. Many industrial areas were also covered: chemical processes, mechatronics, thermal systems and nuclear power plants. On the average each participant knew 8 participants by reputation and 6 participants personally. From that point of view the meeting served a useful purpose in establishing collaborations for future work.

To describe complex systems it is necessary to consider both continuous time and discrete time aspects. The continuous time aspects are described by ordinary or partial differential equations and algebraic equations. One conclusion of the workshop is that it may be possible to unify this aspect of the problem and that differential algebraic equations is the natural framework. There may be very interesting research opportunities in this area; to formulate modeling concepts that can be applied to a wide range of different application fields, to develop software that support the concepts, to develop numerical algorithms for simulating the models based on modular software. The presentations showed clearly that very similar ideas were used in different application areas but with slight differences in terminology and methodology. Clearly much can be gained by a unification. There was a similar situation in 1967 when analog simulation was de facto standardized through the definition of the new Continuous System Simulation Language (CSSL).

The situation is less clear with respect to the discrete time aspects of large systems. This area is less developed although it is very important because of the emerging needs concerning the modeling of hybrid systems. The area has strong connections to computer science and will require much more work.

2. Summary of Presentations

During the two day workshop most of the participants gave presentations on their current and future work. This section gives a short summary of those presentations.

2.1 Karl J. Åström, Lund University, Sweden

Presentation of the COSY program and the goal for the workshop. A brief comment on the state of the art of modeling of complex systems.

2.2 Kaj Juslin, VTT Automation, Finland

Kaj Juslin reported on the work at VTT Automation on process simulation systems. Their current product APROS is a well validated software giving both accurate as well as comprehensive simulations. Major efforts has also been made to make it sufficiently fast to be used for training simulators, for example in the nuclear industry.

Dr. Juslin also reported on their present work on Platform 21, a simulation platform for the 21'st century. It has been used for a number of applications in both power generation and pulp and paper industry. The goal is that P'21 should be able to cooperate with other programs to be used as user interface. The user familiar with AutoCad, G2 etc. should use this as his front-end and have P'21 as a simulation engine in a hidden layer underneath.

2.3 Wolfgang Marquardt, RWTH Aachen, Germany

Wolfgang Marquardt talked about their efforts to support the modeling process, which is seen as a path in a three-dimensional space of model representation, degree of specification and agreement within the modeling team. The path is a creative process were only certain areas are well-known. In Aachen they have created a G2 implementation of a modeling support tool called ModKit. ModKit supports modeling from textual representations to equations and also documents all actions and decisions made during the modeling process so the user can trace actions previously taken and see what were the basic assumptions and decisions made to arrive at a final model.

2.4 Costas Pantelides, Imperial College London, UK

Costas Pantelides gave a comprehensive overview of the process modeling language gPROMS, successor to their dynamic modeling tool SPEEDUP which was sold to Aspen Technologies, Inc 5 years ago. gPROMS is a general purpose process modeling language which is object-oriented to handle large-scale system modeling and model complexity. It allows combined discrete and continuous system modeling and allows the mathematical description to be a combination of algebraic, differential, partial differential and integral equations, IPDAEs. gPROMS features some core applications such as simulation, optimization and three-dimensional visualization, but is also an open architecture which allows for real-time communication with third-party software and applications.

2.5 Bjarne Foss, NTNH Trondheim, Norway

Bjarne Foss presented a graphical language for first principles modeling which had been tested in cooperation with two different industrial users. The results were that the threshold to use modeling in an industrial environment was lowered and that the interaction with process experts was improved. He also reported on an effort to support semi-empirical modeling, i. e., the possibility to combine first-principles models in some operating regimes with other types of models (fuzzy etc.) in other, less well-known operating regimes. This had been implemented in a Matlab toolbox called ORBIT and used in a project together with Daimler-Benz in Germany.

2.6 Sven Erik Mattsson, Lund University, Sweden

Sven Erik Mattsson described in the first half of his talk current activities at his department to develop methods and tools to support model development and use of mathematical models. The projects include development of language constructs for hybrid systems, computational methods, methods for model validation and making reliable model libraries and methods for analysis and extraction of simple models for insight or for control design from complex models. Application areas include thermal power systems and electricity distribution networks.

In the second half of the talk object-oriented modeling of relays and sliding mode behaviour was discussed. Using a relay as an idealized model of a physical phenomena can give rise to a chattering solution with fast switching. However there are several possible ways to define a smooth or so called Filippov solution. Which definition to choose depends on whether the idealized relay represents a continuous gain or a real relay with hysteresis or switching dynamics.

2.7 Serge Steer, INRIA Rocquencourt, France

Serge Steer gave a presentation of the dynamic model builder Scicos which is distributed as a package for their mathematical problem solving software, Scilab. Scicos uses a block-oriented approach to build dynamical systems from predefined libraries with a graphical user interface much like that of Simulink. The main difference is that Scicos can handle state events as well as timed events. The type of mathematical problems supported by Scicos is ordinary differential equations although they are working on implementing support for differential-algebraic equations, DAEs.

2.8 Martin Otter, DLR Oberpfaffenhofen, Germany

Martin Otter had two presentations, one on Friday afternoon and the other on Saturday morning. The first talk concerned object-oriented modeling of multi-body mechanics in Dymola. The approach to model structuring and to get efficient simulation code was outlined. Dymola now supports a library of three-dimensional mechanical components which can be graphically composed into a mechanical system. This software results in simulations that outperforms those from the market-leading commercial package, ADAMS.

Martin Otter's second talk considered a new definition for the perturbation index which describes the numerical properties of a differential algebraic equation (DAE) system. In some cases this is different from the better known differential index which is a mathematical property of the DAE system. Dr. Otter showed that by considering a more structured form of the DAE system where the purely algebraic variables are separated from the differentiated variables the two different indexes will always be the same. Thus you can talk of the *index* of a DAE system.

2.9 Software demonstrations

The last item on Friday's program was software demonstrations. Hilding Elmqvist demonstrated Dymola and the multi-body library previously presented by Martin Otter. He also showed how Dymola could be used to simulate the sound generated by a string or a drum complete with sound output sent to the computer loudspeakers.

Serge Steer showed the dynamic model building package Scicos. The capability of handling state events was shown by a simulation example of a model of a bouncing ball in a two-dimensional room.

Jonas Eborn demonstrated the simulation environment OmSim, developed at the department of Automatic Control, Lund Institute of Technology. He showed how a model database for thermal power systems could be used to build up a model of the heat recovery steam generating system of a combined cycle power plant. This model was then used in a transient simulation of a load change on the power plant.

2.10 Gustaf Söderlind, Lund University, Sweden

Gustaf Söderlind from the Department of Numerical Mathematics presented a generic ODE solving system called Godess. This has been developed at the department since there was a need for a system in which to test different algorithms under *ceteris paribus*, equal terms. A lot of new ODE solving algorithms appear every year but because of differences in implementation comparisons are biased. Godess is an object-oriented method development environment where new algorithms can be implemented easily and tested against well known algorithms. At the moment a large number of Runge-Kutta methods had been implemented, but also a few linear multi-step methods. Godess supports ODEs as well as DAEs and also sparse problems and discontinuities. Although the implementations in Godess are well structured and modular, the loss in efficiency against optimized implementations is less than 20 %.

2.11 Roberto Girelli, Politecnico di Milano, Italy

Roberto Girelli gave a presentation of MOSES, a Modular Object-oriented Software Environment for Simulation. In this project they have focused on using a commercial database, Gemstone, to implement an environment for modeling support. This gives a number of advantages over other modeling environments; data security, team work on common models and traceability of the modeling process. The use of a database creates automatic documentation and relates simulation results to the model version used. The models are defined in an equation based declarative language but the use of a commercial database only allows for partial inheritance, which means that the language can not be fully object-oriented. The simulation environment supports DAEs and hybrid systems and has symbolic manipulation to give efficient simulations. Presently, there are model libraries for two- and three-dimensional mechanics, but there are plans to also build libraries for power generation systems.

2.12 Jan Willems, University of Groningen, the Netherlands

Jan Willems talked about his view on representations of dynamic systems. Key notions are those of *manifest* variables, that can be observed, and *latent* variables, internal to the system. Systems can also be viewed as compositions of subsystems, where the manifest variables are interconnected. Their work has mainly been focused on linear systems, which can be represented by polynomial matrices of the differential operator acting on the variables of the system. The full behavior is described by a set of equations in all the variables and for linear systems this can be reduced to the manifest behavior described by another set of equations in only the manifest variables. Recent results concerning nonlinear systems (multivariate polynomials) show that the reduction property still holds, but the manifest behavior will be described by a set of equations, inequalities and inequations.

2.13 Felix Breitenecker, TU Vienna, Austria

Felix Breitenecker gave a talk for his colleague Prof. Inge Troch who was not able to attend the workshop. The talk considered formulation of design problems in terms of optimization problems. It is important to consider relations between models used and the goals (criteria) to be obtained by the design. Moreover, a designer must also take into account which tools he has available. It is of no use for him to formulate an optimization problem which he cannot solve.

2.14 Adolf Glattfelder, ETH Zürich, Switzerland

Adolf Glattfelder gave a more practical view on modeling than in the other presentations. He had been involved in a project to give support for using models in engineering work in small companies and presented a design study on a hydraulic positioning system for a hydro turbine gate valve. In this project they had used a four-phase modeling procedure consisting of data collection, qualitative modeling, quantitative modeling and state space description. From the control specifications and plant data they deduced three models of increasing complexity. The modeling was done by engineering work but the fourth phase was supported by manipulations in Maple. From this they proceeded with control design on the three models and could show that the PI-controller designed with the first-order model was not sufficient (unstable) and designed a feedback controller that fulfilled the specifications for the high-order model.

2.15 Miquel Piera, Universitat Autònoma de Barcelona, Spain

Miquel Piera spoke about PMT, the physical modeling tool, that can be used to build and simulate models of chemical processes. The idea is to have a predefined model library of process units like valves, tanks etc. The user picks units from a menu and builds up the model topology with graphical icons. This topology can then automatically be translated into an equation system, using physical knowledge that is coded into the predefined unit models. This knowledge is also used to remove algebraic loops that occur when resistances are connected in series. Unnecessary equations can also be removed by the user placing sensors into the flowsheet, thus indicating what variables are interesting for the simulation.

At the moment PMT produces ACSL code for simulations, but there are plans to introduce the possibility to produce Dymola code. In the PMT environment there are also possibilities to do linearization and validation of models by simulation.

2.16 Antoni Guasch, Politècnica de Catalunya, Barcelona, Spain

Antoni Guasch presented his view on the modeling and simulation life cycle, applied to a project study on a nuclear tertiary cooling system. His work concerned the modeling process or life cycle, touching on similar issues as Wolfgang Marquardt. The point was that the actual modeling work amounted to a very small part of the entire project, around 15%, while the major part of the work was spent on verification, validation and documentation of the model and the simulations made. Documents concerning specifications and results quickly become so numerous that the information is difficult to grasp. Furthermore, consistency is an issue. There is a need for some kind of database support for the different phases in a modeling project, including producing and maintaining the documentation needed.

2.17 Hilding Elmqvist, Dynasim, Sweden

Hilding Elmqvist reported from a newly started effort to design a unified object-oriented modeling language. The effort is a part of the Simulation in Europe (SiE), which is a basic research project within the ESPRIT programme. There is only funding for travel costs.

The long range goal is to design a multi-formalism, multi-domain, general-purpose modeling language. The work will start in the continuous corner since there is a common mathematical framework in the form of differential-algebraic equations (DAEs) and there are a number of existing modeling languages based on similar ideas, such as Dymola, gPROMS, MOSES, NMF, OMOLA and U.L.M. Furthermore, there is quite a vast experience of using them for various applications. It thus seems to be appropriate to collect all knowledge and experience and design a new unified model language or neutral format for model representation. Modeling of discrete event system is very heterogeneous and not that well-understood. Thus, the effort has begun by defining a new modeling language called *Modelica* for DAE systems. This will be extended with some discrete event features to handle discontinuities and sampled systems.

It is necessary to promote research and evolution. The language should be open to allow additions of more informations to models to define purpose, diagnostic support, etc. The base language must be complete, i.e., be able to describe models and it must be possible to extend it in certain, well-defined ways to allow evolution, research and innovation. When experiences of new extensions are gained and they become mature, they can be standardized.

3. Conclusions

There were intense discussions during and after the presentations, at coffee breaks and at the workshop dinners. There was also a separate discussion session. The conclusions drawn can be summarized as follows:

1. A methodology for modeling complex systems is needed. The methodology should be based on a firm theoretical foundation and should be supported by appropriate software including modeling and experiment environments. Modeling environment: creation, deletion, storage, change and exchange, visualization, transformation etc. of models, layers (OSI) of models. Experiment environment: simulation, optimization, symbolic manipulation, linearization, and exploration of models.
2. Differential algebraic equations and the theory of behavioral systems is a good foundation. Much work remains before the theory is fully developed.
3. Current modeling practice is inadequate for two main reasons. Modeling is tightly integrated with simulation and it is based on ordinary differential equations. This approach does not permit the development of model libraries. It is also difficult to apply symbolic reasoning because the models are not represented on a form that permits this.
4. There are a number of emerging modeling languages which form a good basis for future work for example gPROMS, ANDECS, Dymola, OMOLA, Scicos, MOSES, PMT, NMF, U.L.M., DEVS. They have been applied to chemical processes, multi-body systems, mechanical, electrical, thermal and hydraulic systems.
5. Many emerging methods are based on object oriented analysis and design techniques. This approach appears well suited to modeling of complex systems. Models of complex systems are naturally organized in hierarchies with "is-a", "consists-of" and "uses" connections. In spite of similarities of the emerging approaches there are also many differences. There are particularly large differences in terminology and notation. There is a strong need for unification of methods and notations.
6. There are interesting developments in numerical mathematics that could be exploited. These results should be encapsulated in modular software. Further development of solvers for DAEs and IPDAEs are needed.
7. Much work on software is required. Model-view concept from computer science may be useful. In this concept a model is viewed as a persistent object in an object-oriented database with several views, for example equations, diagrams and responses. The database should have automatic facilities for updating views when a model is changed.
8. When dealing with complex systems it is necessary to deal with both their continuous time and discrete time aspects. The continuous time aspects are relatively well understood but much work remains with respect to discrete time aspects.

Several experimental systems support this although there is a strong need for unification of methods and algorithms. There is also a strong need for development of appropriate numerical methods and software.

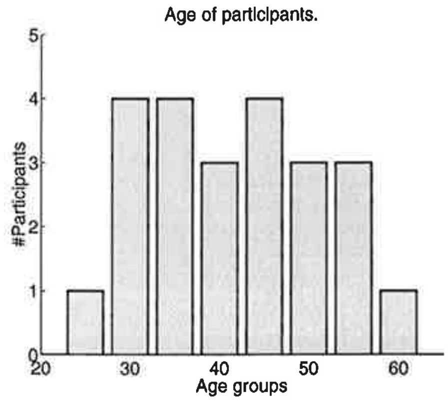

Figure 1 Histogram of the age distribution of the participants.

4. Workshop Survey

The workshop had 23 participants, in addition there were 2 graduate students who helped with local arrangements. Most invited participants were able to come. The age distribution of the participants is shown in Figure 1.

The relations between the participants are illustrated in Figure 2 which shows the statistics of how many of the other participants each one knew personally and by reputation. It is very interesting to see how many participants that had not met previously.

After the workshop the participants was asked to answer a few questions about the workshop. The questions were:

1. How old are you?
2. Before the meeting, how many of the participants did you know only by reputation?
3. Before the meeting, how many of the participants did you know personally?
4. What is your research field/speciality?
5. Rate the relevancy of the meeting to your research. 0 = useless, 10 = very useful.

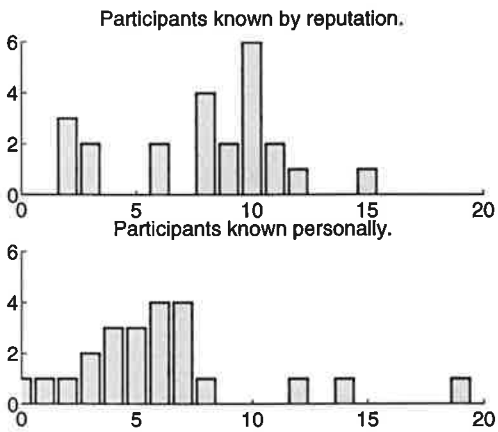

Figure 2 Histogram of personal relations between the participants.

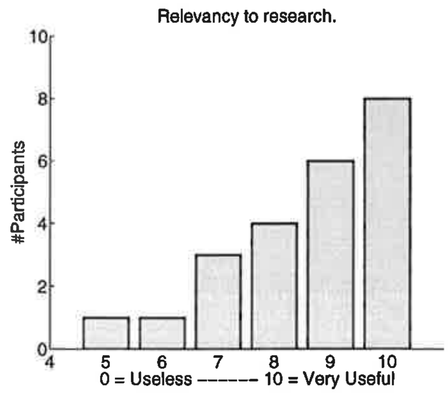

Figure 3 Histogram of the participants opinion of the workshop.

The results to the questions 1, 2 and 3 are summarized in Figures 1-2.

The answers to question 4 varied, but the common denominators seem to be:

- Object-Oriented and Physical Modeling
- CACSD tools and software
- Process control
- Systems theory
- Numerical methods and analysis

The answers to the last question are summarized in Figure 3. As a conclusion, all the participants at the workshop seemed to agree that it was a successful and very rewarding event. This was also the general feeling at the closing discussions and workshop dinners. In summary we felt that the meeting was a good forum for bringing a small group of active researchers together to advance the approaches to modeling of complex systems.

List of Participants

COSY Workshop on Mathematical Modeling of Complex Systems
Lund, Sweden, September 1996

Beukers, Paula
University of Groningen
Mathematics Institute
P.O. Box 800
9700 AV Groningen
THE NETHERLANDS

Phone +31-503639111
Fax +31-503633976
E-mail paula@math.rug.nl

Breitenecker, Felix
Technische Universitaet Wien
Abt. Simulations-Technik
Wiedner Hauptstrasse 8-10
A-1040 Wien
AUSTRIA

Phone +43-1588015374, 5386
Fax +43-15874211
E-mail felix.breitenecker@tuwien.ac.at

Eborn, Jonas
Lund Institute of Technology
Dept of Automatic Control
Box 118
221 00 Lund
SWEDEN

Phone +46 46-2228784
Fax +46 46-138118
E-mail Jonas.Eborn@control.lth.se

Elmqvist, Hilding
Dynasim
Forskningsbyn IDEON
222 70 Lund
SWEDEN

Phone +46 46-182500
Fax +46 46-129879
E-mail Elmqvist@Dynasim.se

Foss, Bjarne
Norwegian University of Science and Technology
Dept. of Engineering Cybernetics
N 7034 Trondheim
NORWAY

Phone +47-73594476
Fax +47-73594399
E-mail Bjarne.Foss@itk.unit.no

Girelli, Roberto
Politecnico di Milano
Dept. Elettronica e Informazione
Piazza Leonardo da Vinci 32
20133 Milano
ITALY

Phone +39-223993669
Fax +39-223993412
E-mail girelli@elet.polimi.it

Glattfelder, Adolf
Automatic Control Laboratory
ETH-Zentrum
CH-8092 Zurich
SWITZERLAND

Phone +41-16325300
Fax +41-16321211
E-mail glatt@aut.ee.ethz.ch

Guasch, Antoni
Universitat Politecnica de Catalunya
Department ESAII - ETSEIT
Colom 11
08222 Barcelona
SPAIN

Phone +34-3 7398144
Fax +34-3 7398101
E-mail guasch@esaii.upc.es

Juslin, Kaj
VTT Automation
Technical Research Centre of Finland
P.O. Box 1301
Fin-02044 VTT
FINLAND

Phone +358-94566422
Fax +358-94566475
E-mail Kaj.Juslin@vtt.fi

Maffezzoni, Claudio
Politecnico di Milano
Dept. Elettronica e Informazione
Piazza Leonardo da Vinci 32
20133 Milano
ITALY

Phone +39-223993616
Fax +39-223993587
E-mail maffezzo@elet.polimi.it

Marquardt, Wolfgang
Lehrstuhl fur Prozesstechnik
Technische Hochschule Aachen
Rheinisch-Westfälische
52064 Aachen
GERMANY

Phone +49-241806712
Fax +49-2418888326
E-mail maq@lfpt.rwth-aachen.de

Mattsson, Sven Erik
Lund Institute of Technology
Dept. of Automatic Control
Box 118
22100 Lund
SWEDEN

Phone +46 46-2228779
Fax +46 46-138118
E-mail Sven_Erik.Mattsson@control.lth.se

Möllerstedt, Erik
Lund Institute of Technology
Dept of Automatic Control
Box 118
221 00 LUND

Phone +46-462223270
Fax +46-46138118
E-mail erik.mollerstedt@control.lth.se

Navarro, Jose Luis
Universidad Politecnica de Valencia
Dep. Ing. de Sistemas, Computadores y Automatica
P.O. Box 22012
46071 Valencia
SPAIN

Phone +34-63877576
Fax +34-63879579
E-mail joseluis@aii.upv.es

Nilsson, Bernt
Lund Institute of Technology
Dept. of Automatic Control
Box 118
221 00 Lund
SWEDEN

Phone +46-46 2228784, 2223627
Fax
E-mail Bernt.Nilsson@control.lth.se

Otter, Martin
DLR Oberpfaffenhofen
Institut fuer Robotik und Systemdynamik
D-82234 Wessling
GERMANY

Phone +49-8153282473
Fax +49-8153281441
E-mail Martin.Otter@dlr.de

Pantelides, Costas
Imperial College of Science,
Techn. and Medicine Centre for Process Syst. Eng.
London SW7 2AZ
UNITED KINGDOM

Phone +44-1715946622
Fax +44-1715946606
E-mail c.pantelides@ic.ac.uk

Piera, Miquel Angel
Universitat Autonoma de Barcelona
Computer Science Department
Facultat de Ciencies
08193 Bellaterra
SPAIN

Phone +34-35811360
Fax +34-35813033
E-mail miquel@sunaut.uab.es

Rapisarda, Paulo
University of Groningen
Mathematics Institute
P.O. Box 800
9700 AV Groningen
THE NETHERLANDS

Phone +31-503639111
Fax +31-503633976
E-mail paulo@math.rug.nl

Schaufelberger, Walter
ETH-Zurich ETL
Inst. für Automatic
ETH Zentrum
CH-8092 Zurich
SWITZERLAND

Phone +41 1 632 4190
Fax +41-16321211
E-mail ws@aut.ee.ethz.ch

Steer, Serge
INRIA
Institut National d'Informatique et Automatique
78153 Le Chesnay Cedex
FRANCE

Phone
Fax
E-mail Serge.Steer@inria.fr

Söderlind, Gustaf
Lund University
Numerical Mathematics
Box 118
221 00 Lund
SWEDEN

Phone +46 46 2224909
Fax +46 46-131021
E-mail Gustaf.Soderlind@dna.lth.se

Willems, Jan
University of Groningen
Dept. of Mathematics
P.O. Box 800
NL-9700 AV Groningen
THE NETHERLANDS

Phone +31-50 3633984
Fax +31-50 3633976
E-mail j.c.willems@math.rug.nl

Åström, Karl Johan
Lund Institute of Technology
Department of Automatic Controll
Box 118
221 00 Lund
SWEDEN

Phone +46 46-2228781
Fax +46 46-138118
E-mail Karl_Johan.Astrom@control.lth.se

Öhman, Martin
Lund Institute of Technology
Dept of Automatic Control
Box 118
221 00 LUND

Phone +46-462220362
Fax +46-46138118
E-mail martin.ohman@control.lth.se

Final program for the COSY Workshop on Mathematical Modeling of Complex Systems in Lund, September 5-7, 1996

Thursday September 5

19.30 DINNER at Grand Hotel

Friday September 6

9.00 Welcome
COSY Program and Workshop Goals,
K.J. Åström
9.30 A companion model approach for simulation of large complex systems,
K. Juslin

10.15 COFFEE

10.30 Recent progress in computer-aided modelling at RWTH Aachen,
W. Marquardt
11.15 An overview of hybrid system modelling in gPROMS,
C.C. Pantelides

12.00 LUNCH

13.00 Modeling methods for first principles and semi-empirical models,
B.A. Foss
13.45 Modelling and simulation of hybrid complex systems,
S.E. Mattsson
14.30 Scicos, a hybrid system simulator: methodology and implementation,
S. Steer

15.15 COFFEE

15.45 Object-oriented modelling of multi-body systems,
M. Otter
16.30 Demonstrations of Dymola, OmSim and Scicos
18.00 CLOSING

19.30 DINNER at Kulturen's Restaurant

Saturday September 7

9.00 A constructive definition of the perturbation index,
M. Otter
9.30 Godess -- a generic ODE solving system in C++,
G. Söderlind

10.15 COFFEE

10.30 Data Models for object-oriented modelling and simulation,
C. Maffezzoni and R. Girelli
11.15 System representations and LQ and H-infinity problems,
J. Willems

12.00 LUNCH

13.00 Modelling for optimal control,
F. Breitenecker
13.45 Systematic modelling for control: An electrohydraulic actuator system,
W. Schaufelberger and A.H. Glattfelder
14.30 Modelling Tools in PMT to Evaluate Control Performance
in the Process Industry,
M. Angel Piera

15.15 COFFEE

15.45 Study of the tertiary cooling system of a nuclear power station:
Modelling and simulation life cycle,
A. Guasch
16.30 An Effort to Design of a Unified Object-Oriented Modeling
Language. The ESPRIT project: Simulation in Europe Basic Research
Working Group (SiE-WG),
H. Elmqvist
17.15 DISCUSSION
18.00 CLOSING

19.30 DINNER at Petri Pumpa

Each contribution is given 30 minutes for presentation and 15 minutes for questions and discussion.