Mathematical Modelling

Syllabus for a Master Course

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1 General goals of the course

This course should provide an introduction into the wide and diverse field of mathematical modelling in various application areas. Following an introduction into basics respectively into the "philosophy" of mathematical modelling the presentation is done by considering concrete examples of modelling processes intertwined with modules presenting mathematical methodologies. The goal of this organization of the course material is twofold:

a) After attending the course it should be clear that mathematical modelling of concrete problems is to a high degree interdisciplinary and can only be done in collaboration with scientists in the application field. It furthermore requirers that the mathematician is familiar with the basic facts of the applied problem. Moreover, in order to conduct modelling processes successfully the mathematician has to have a clear view of the goals related to the process in the application area.
b) It should be obvious that mathematical modelling needs a wide spectrum of mathematical tools dependent on the concrete problem under consideration.

In view of goal a) from above it is recommended that the course will be modified in the future in order to incorporate examples from application fields represented at the partner universities.

2 Overview on the course modules

We first list the modules of the course and present subsequently the educational goals of these modules.

Table: Modules of the course

PART I: Basics, Parameter Estimation and Regression Models (30 units)

Module	No. of units	Contents
I: Basics of Mathematical Modelling	3	Types of models. Goals of a modelling process. Guidelines for a modelling process. The domain of validity of a model. The role of mathematicians in a modelling process.
II: Dimensional Analysis	4	Physical dimensions and units. Buckingham's π-Theorem. Examples.
III: The Bromsulphalein Retention Test	5	Description of the test. Compartment model for the test. Basic assumptions for compartment models. Formulation of the parameter estimation problem as an optimization problem. Computational issues.
IV: Parameter estimation and sensitivity analysis	8	Formulation of the least squares estimation problem. Statistical properties of the least squares estimator. Sensitivity analysis.
V: Regression Models	10	Introduction into probabilistic concepts (probability space, random variable, expected value, variance etc.). Simple and multiple regression analysis. Introduction to maximum-likelihood estimation. Typical examples.

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PART II: Enzyme Kinetics, Predator-Prey Interactions and PDE-Models (30 units)

VI: Enzyme Kinetics	5	Enzymatic reactions, lock and key concept. Derivation of the model on the basis of the "law of mass action". Michaelis-Menten resp. Briggs-Haldane approximation. Introduction of dimensionless variables and explanation of the Michaelis-Menten approximation via a singularly perturbed system.
VII: Interacting Populations	5	Basic assumptions in order to develop an ODE-model for the two interacting populations and derivation of corresponding models. Models for prey-predator interaction and models in epidemics. Basic properties of such models (equilibria, invariance of the positive cone), phase plane concept. Proof for the existence of periodic solutions.
VIII: Conservation laws	13	Basic assumptions for conservation laws, constitutive relations. Basic facts on the method of characteristics for quasilinear first order PDEs. Examples: Age dependent population models, traffic flow models.
IX: Three-Dimensional Vibrations of a String	7	Formulation of assumptions and derivation of the model (d'Alembert's law). Small vibrations (i.e., under what conditions can the three model equations be decoupled into three linear wave equations).
Total no. of units:	**60**	

3 Educational goals of the modules

3.1 Module I

This module should provide an introduction to some basic facts concerning mathematical modelling. In particular, students should get an overview concerning possible goals of a modelling process and concerning guidelines which have to be observed in a modelling process.

3.2 Module II

Mathematicians in general are not used to consider physical dimensions and units. Therefore it is necessary to introduce students into this field. Buckingham's π-Theorem is an important tool to get fundamental relations between the physical quantities in a modelling process. Examples should demonstrate this.

3.3 Module III

This module should introduce the concept of compartment models for a very simple situation. Moreover, it should demonstrate one possible goal of a modelling process: to determine a quantity (here the decay rate of bromsulphalein in the liver) which cannot measured directly. This involves estimation of parameters in the model. Therefore the frequently used formulation of the parameter estimation problem as an optimization problem is also introduced as an preparation for the next module.

3.4 Module IV

This module should introduce the students to the basic facts on the least squares estimator. In addition, some basic fact on sensitivity analysis should be introduced.

3.5 Module V

Most of the modules of this course deal with so called explanatory models, i.e., models which reflect the causal relations, which are governing the real system. Regression models can be considered to be descriptive. It is very important that the students also get some basic fact about this important class of models and the corresponding statistical background.

3.6 Module VI

The Michaelis-Menten approximation is frequently used for modelling enzymatic reactions. In this concrete case the so called "law of mass action" is introduced, which is the basis for many modelling processes involving chemical reactions. Furthermore, with this example one can demonstrate the usefulness of introducing dimensionless quantities.

3.7 Module VII

This module is representing a class of models frequently used in population dynamics and dynamics of diseases. The mathematical discussion of the model is based on the phase plane concept, which is used frequently for two dimensional autonomous systems.

3.8 Module VIII

For many concrete situations the modelling process is based on the considerations of quantities which are conserved. The characteristics of the concrete situation are reflected by the constitutive laws, which have to be obtained. The use of this approach is demonstrated by models for age-structured populations and for traffic flow.

3.9 Module IX

The derivation of the model in this case is rather typical for problems in mechanics (application of d'Alembert's law). The problem of small solutions should demonstrate that neglecting higher order terms has to be done with caution.

4 Literature

4.1 Module I

R. Aris: Mathematical Modelling Techniques,
Research Notes in Mathematics Vol. 24, Pitman, London 1978.

H. T. Banks: Modeling and Control in the Biomedical Sciences,
Lecture Notes in Biomathematics Vol. 6, Springer-Verlag, Berlin 1975.

H. T. Banks and H. T. Tran: Mathematical and Experimental Modeling of Physical and Biological Processes, CRC PRESS, Boca Raton 2009.

A. Beuter, L. Glass, M. C. Mackey, and M. S. Titcombe (Editors): Nonlinear Dynamics in Physiology and Medicine, Springer Verlag, Berlin 2003.

Y. Cherruault: Mathematical Modelling in Biomedicine: Optimal Control of Biomedical Systems, D. Reidel Publ., Dordrecht 1986.

C. L. Dym and E. S. Ivey: Principles of Mathematical Modeling,
Academic Press, New York 1980.

L. Edelstein-Keshet:Mathematical Models in Biology,
SIAM, Philadelphia 2005.

T. L. Saaty and J. M. Alexander: Thinking with Models,
Pergamon Press, Oxford, 1981.

4.2 Module II

E. Buckingham: *On physically similar systems; illustrations of the use of dimensional equations*, Phys. Rev. **4**(1914), 345 – 376.

H. Hanche-Olsen: *A note on Buckingham's π-theorem*, www.math.ntnu.no/∼hanche/notes/buckingham/, 2001.

H. E. Huntley, Dimensional Analysis, Dover Publications, New York 1967.

4.3 Module III

U. Feldmann and B. Schneider: *A general approach to multicompartment analysis and models for the pharmacodynamics*, in "Mathematical Models in Medicine" (J. Berger, W. Bühler, R. Repges and P. Tautu, eds.), pp. 243 – 279, Lecture Notes in Biomathematics Vol. 11, Springer-Verlag, Berlin 1976.

4.4 Module IV

G. A. F. Seber and C. J. Wild: Nonlinear Regression, John Wiley & Sons, New York 1989.

V. G. Voinov and M. S. Nikulin: Unbiased Estimates and Their Applications, Vol. 1: Univariate Case, Vol. 2: Multivariate Case, Kluwer Academic Publ., Dordrecht 1993, 1996.

4.5 Module V

C. Chatfield: The Analysis of Time Series, An Introduction, 6th edition, Chapman & Hall, Boca Raton 2004.

C. R. S. Dougherty: Introduction to Econometrics (3rd edn.), Oxford University Press, Oxford 2006.

H. Madsen: Time Series Analysis,Chapman & Hall/CRC, Boca Raton 2008.

J. F. Monahan: A Primer on Linear Models, Chapman & Hall, Boca Raton 2008.

4.6 Module VI

J.-P. Kernevez: Enzyme Mathematics, North Holland Publ., Amsterdam 1980.

S. I. Rubinow: Mathematical Problems in the Biological Sciences, CBMS Vol. 10, SIAM, Philadelphia 1973.

4.7 Module VII

D. J. Daley and J. Gani, Epidemic Modelling: An Introduction, Cam- bridge Studies in Mathematical Biology Vol. 15, Cambridge University Press, Cambridge 1999.

H. I. Freedman: Deterministic Mathematical Models in Population Ecology, Marcel Dekker, New York 1980.

N. S. Goel, S. C. Maitra, and E. W. Montroll: Nonlinear Models of interacting Populations, Academic Press, New York 1971.

4.8 Module VIII

F. A. Haight, Mathematical Theories of Traffic Flow, Academic Press, New York 1963.

J. W. Sinko and W. Streifer: *A new model for age-size structure for a population*, Ecology **48** (1967), 910 – 918.

4.9 Module IX

V. I. Babitsky and V. L. Krupenin: Vibrations of Strongly Nonlinear Systems, Springer Verlag, Berlin 2001.

A. Klarbring: Models of Mechanics, Springer Verlag, Berlin 2006.

M. Levi: The Mathematical Mechanic: Using Physical Reasoning to Solve Problems, Princeton University Press, Princeton (NJ) 2009.

N. S. Ottosen and M. Ristinmaa: The Mechanics of Constitutive Modeling, Elsevier, Amsterdam 2005.

R. Temam and A. Miranville: Mathematical Modeling in Continuum Mechanics, Cambridge University Press, Cambridge 2001.

5 Teaching

The course should be accompanied by homework exercises which should require at most 2 of the afternoon sessions as indicated below. The major part of the afternoon session should be spent by working independently in teams on modeling projects . The results also should be presented in the afternoon sessions. During the afternoon session the teacher should be available for questions respectively be present in order to get an impression on performance of the students.

The course is planned for 4 weeks, each week from Monday till Friday. This implies that there will be 3 teaching units (45 minutes) per day. The following schedule is proposed for each day:

8:00 till 11:00:	three units with breaks in between;
11:30 till 12:30:	discussion with the teacher;
15:00 till 17:30:	work on homework exercises, work in teams on problems posed by the lecturer, presentation of results, respectively

6 Grading

The basis for grading is provided by the performance of students in the following items:

a) Exercises for *homework* will be regularly given in order to provide possibilities for a better understanding of the material presented in the course.
b) During each week of the course a *modeling project* should be performed by the students in teams of 4 – 5 persons. The results obtained have to be presented by the teams.
c) An *oral examination* concerning the course.

The oral examination could consist of several parts taken at different times and should give the lecturer an impression on how well the student has understood the material of the course.

In order to obtain the grade for the course the following weights will be used for the items a) – c) from above:

Homework exercises	20%
Modeling projects	50%
Oral examination	30%