Simulation Foundations, Methods and Applications

David J. Murray-Smith

Testing and Validation of Computer Simulation Models

Principles, Methods and Applications



Simulation Foundations, Methods and Applications

Series Editor

Louis G. Birta, University of Ottawa, Canada

Advisory Board

Roy E. Crosbie, California State University, Chico, USA Tony Jakeman, Australian National University, Australia Axel Lehmann, Universität der Bundeswehr München, Germany Stewart Robinson, Loughborough University, UK Andreas Tolk, Old Dominion University, USA Bernard P. Zeigler, University of Arizona, USA More information about this series at http://www.springer.com/series/10128

David J. Murray-Smith

Testing and Validation of Computer Simulation Models

Principles, Methods and Applications



David J. Murray-Smith School of Engineering University of Glasgow Glasgow, UK

 ISSN 2195-2817
 ISSN 2195-2825
 (electronic)

 Simulation Foundations, Methods
 and Applications

 ISBN 978-3-319-15098-7
 ISBN 978-3-319-15099-4
 (eBook)

 DOI 10.1007/978-3-319-15099-4

Library of Congress Control Number: 2015953011

Springer Cham Heidelberg New York Dordrecht London © Springer International Publishing Switzerland 2015

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made.

Printed on acid-free paper

Springer International Publishing AG Switzerland is part of Springer Science+Business Media (www.springer.com)

Preface

This book is intended to fill a gap in the currently available literature on the development and application of dynamic simulation models. It deals with issues of model quality and, more specifically, with the processes of testing, verification and validation. Since simulation models can never be proved to be "valid" in any absolute sense, the topic of model testing inevitably involves subjective issues and often a trade-off between accuracy, cost and practical issues associated with the intended application of the model. The emphasis within the book is mainly on continuous system simulation problems, and case studies are used to provide examples from the fields of engineering and physiology. The range of these applications and their cross-disciplinary nature reflects my research interests and activities over a period of almost 50 years.

Since the book is aimed at people with interests in simulation models and their use in practical applications in many different fields, some assumptions are made about the prior knowledge of the readers. Relevant supplementary material is therefore being provided through a website (http://www.springer.com/gb/book/ 9783319150987), and it is hoped that this should provide a convenient way of accessing additional background information, both in terms of the general principles of modelling and the application areas considered in the case studies. For those who do not have a background in engineering and the physical sciences, this includes sections about mathematical and system modelling concepts. Similarly, for those whose prior knowledge is lacking in terms of the biological sciences and who need more in order to understand aspects of some of the physiological case studies, the supplementary material includes sections which present some basic concepts from those areas. No attempt has been made to make the supplementary material sufficient on its own to meet the needs of everyone. Instead, only a brief account of each topic is included on the website, and links are provided to other sources of information which are far more extensive and detailed. The supplementary material also includes some data sets relating to some of the case studies, and it is hoped that these may allow readers to carry out their own investigations of those examples. Frequency-domain and time-domain data from tests carried out on some relatively simple systems and models, which are not discussed within the book, are also provided. It is hoped that these may allow the reader to explore and apply experimental modelling and model testing methods to these additional data sets. All the data sets and models provided through the website may be used freely and shared with others, provided the source is acknowledged.

Since the case studies, and other applications discussed in the book, are drawn from research projects and my teaching activities, I must record my sincere thanks to the many research students, research assistants, undergraduate students and colleagues who contributed in important ways. Some of those receive explicit mention through references to reports, theses and journal or conference publications, but I must express my thanks to all who have contributed to the work in any way. I must also thank students who may have encountered some of these case studies within their courses and whose questions and difficulties have contributed significantly to the way in which material has been presented.

Glasgow, UK June 2015 David J. Murray-Smith

Contents

1	An Introduction to Simulation Models and the Modelling Process					
	1.1	Objectives in Mathematical Modelling				
		and Computer Simulation	1			
	1.2	Requirements Definition and Conceptual Modelling	3			
	1.3	Issues of Model Quality	5			
	1.4	Model Re-use	6			
		1.4.1 Model Libraries	6			
		1.4.2 Generic Models	7			
	1.5	Classes of Model	8			
		1.5.1 Models Involving Continuous Variables	9			
		1.5.2 Discrete-Event and Hybrid Models	11			
		1.5.3 Inverse Models and Inverse Simulation Methods	12			
	1.6	Interactions Between Different Types of Simulation Model				
		and Other Software Tools	14			
	1.7	Organisation of the Book	14			
	Refe	rences	16			
2	Conc	Concepts of Simulation Model Testing, Verification				
	and	Validation	19			
	2.1	Model Quality, Uncertainties and Errors	19			
	2.2	The Iterative Processes of Model Development,				
		Testing, Improvement and Acceptance	23			
	2.3	The General Principles of Model Evaluation	28			
	2.4	Verification and Validation of Sub-models	30			
	2.5	Discussion	31			
	Refe	rences	32			
3	Meas	sures of Quality for Model Validation	35			
	3.1	Choice of Output Variables for Model Quality Assessment	35			
	3.2	Graphical Methods and Measures	36			

	3.3	Determ	ninistic Quantitative Measures	39
		3.3.1	Time-Domain Measures	39
		3.3.2	Frequency-Domain Measures and Comparisons	43
	3.4	Statisti	cal Measures	44
	3.5	Visuali	isation Techniques	45
		3.5.1	Polar Diagrams	45
	Refer	ences		47
4	Sensi	tivity A	nalvsis for Model Evaluation	49
	4.1	An Inti	roduction to Sensitivity Analysis Methods	49
	4.2	Sensiti	vity Functions	50
		4.2.1	Parameter Perturbation Methods	
			of Sensitivity Analysis	51
		4.2.2	Sensitivity Analysis Through the Use of Sensitivity	
			Models	52
	4.3	Parame	eter Sensitivity Analysis of Linearised Continuous	
		State-S	pace Models	54
	4.4	Parame	eter Sensitivity Analysis of Continuous	
		Transfe	er Function Models	55
	4.5	Sensiti	vity Analysis and Validation of Continuous Models	
	1.6	for Sm	all and Large Changes in the System	56
	4.6	Sensiti	vity Analysis of Discrete-Event and Hybrid Models	58
	4./	Discus	sion	59
	Refer	ences		39
5	Expe	rimenta	l Data for Model Validation	61
	5.1	An Inti	roduction to Experimental Modelling Techniques	61
	5.2	Experi	mental Modelling Methods and Their Role in Model	
		Develo	ppment and Validation	63
		5.2.1	An Overview of System Identification and Parameter	
			Estimation Techniques	64
		5.2.2	Model Structure Optimisation	66
		5.2.3	Issues of Identifiability	69
		5.2.4	Design of Experiments and the Selection	71
		5 2 5	A company of Estimates	71
	Dafar	5.2.5	Accuracy of Estimates	74
	Keler	ences		73
6	Meth	ods of N	Model Verification	77
	6.1	Genera	Il Issues in Simulation Model Verification	77
		6.1.1	Verification of Simulation Models Based on Ordinary	
			Differential Equations and Differential Algebraic	
		(10)	Equations	80
		6.1.2	Verification of Models Based on Partial Differential	
			Equations	81

		6.1.3 Verification of Discrete-Event and Hybrid Models	81
	6.2	The Role of Formal Methods in the Verification of Simulation	
		Models	82
	Refere	ences	83
7	Meth	ods for the Invalidation/Validation of Simulation Models	85
	7.1	An Introduction to Methods of Model (In)Validation	85
	7.2	Ouantitative Methods	86
		7.2.1 Simple Methods for Predictive Validation	86
		7.2.2 Methods Involving System Identification	
		and Parameter Estimation Techniques	88
		7.2.3 Barrier Certificate Methods	92
		7.2.4 Methods Based on Model Distortion	92
		7.2.5 Methods Based on Parameter Sensitivity Analysis	94
	7.3	Face Validation	95
	7.4	Approaches Based on Comparisons with Other Models	101
	7.5	Data Sets for Model Testing	102
	7.6	Validation of Sub-models and Generic Models	104
		7.6.1 Library Sub-models	104
		7.0.2 Generic Models	105
	1.1	Volidation of Disorate Event and Hybrid Models	105
	7.8	A acentance or Unorading of Models	100
	7.9	Discussion	100
	7.10 Refer	Discussion	107
	Kelen		109
8	Mana	gement Issues Within Simulation Model Development	
	and T	Sesting	113
	8.1	The Need for Management Procedures	113
	8.2	Tools for the Management of Simulation Models	117
	8.3	Simulation Model Documentation and the Use	
		of Model Libraries	117
	8.4	Benefits Versus Costs of Model Management Procedures	121
	Refere	ences	124
9	Case	Study: Development and Testing of a Simulation Model	
	of Tw	o Interconnected Vessels	127
	9.1	Introduction to the Case Study	127
	9.2	A Nonlinear Model of the Coupled-Tanks System	128
	9.3	Experiments for Estimation of Parameters C_{d1} and C_{d2}	131
		9.3.1 A Test for Estimation of the Discharge	
		Coefficient C_{dl}	131
		9.3.2 A Test for Estimation of the Discharge	
		Coefficient C_{d2}	132

		9.3.3 I	Estimation of Coefficients C_{d1} and C_{d2} from	
		-	Test Results for Steady-State Conditions	133
	9.4	Internal V	Verification of the Simulation Model	134
		9.4.1 \$	Systematic Checking of Code or Block Diagram	
		I	Interconnections	134
		9.4.2	Algorithmic Checks	135
		9.4.3	Checks Involving Comparisons of Simulation	
		I	Results with Analytical Solutions	135
	9.5	Validatio	on of the Simulation Model	136
		9.5.1 (Graphical Methods	137
		9.5.2	Application of the Model Distortion Approach	139
		9.5.3	Application of Genetic Programming (GP)	
			Techniques	141
		9.5.4	Application of the Inverse Simulation Approach	142
	9.6	Possible	Improvements to the Basic Model	144
	Refer	ences	r	145
10	Case	Study: M	odel Validation and Experiment	
	Desig	n for Heli	copter Simulation Model Development	
	and A	Application	ns	147
	10.1	Problem	Areas in Helicopter Modelling and Simulation	147
		10.1.1	Quantitative Criteria for Functional Validation	
		(of Helicopter Models	148
		10.1.2 I	Investigation of Physical Fidelity in Helicopter	
		9	Simulation Models	149
	10.2	System Id	dentification and Parameter Estimation in	
		Helicopte	er Modelling	150
		10.2.1 I	Equation-Error Estimators	154
		10.2.2	Output-Error Estimators	155
		10.2.3 I	Maximum-Likelihood Estimators	156
	10.3	Test Inpu	it Design for Helicopter System Identification	
		and Mode	el Validation	157
		10.3.1 l	Design for a Specified Input Auto-spectrum	160
	10.4	The Valio	dation of Six-Degrees-of-Freedom	
		Helicopte	er Models	165
	10.5	Coupled	Flapping/Inflow Models of Helicopter Rotors	170
	10.6	Discussic	on	170
	Refer	ences		172
11	Case	Study: Co	ompartmental Modelling of the Gas-Exchange	
	Proc	esses of the	e Human Lungs	175
	11.1	Introduct	ion	175
		11.1.1	Modelling and Simulation Techniques	
		i	in Respiratory Physiology	176

Contents

	11.2	Simple	Compartmental Models with Continuous Gas	177		
		and Blo		1//		
		11.2.1	General Case for Gases That Are Soluble in Blood	1/8		
		11.2.2	Case of Insoluble Inert Gases	180		
		11.2.3	Issues of Model Quality in Models with Continuous			
			Ventilation and Perfusion	180		
	11.3	A Com	partmental Model with Tidal Breathing	181		
		11.3.1 11.3.2	A Tidal-Ventilation Model for Carbon Dioxide Identifiability Analysis of the Gas Exchange Model	184		
			for Carbon Dioxide	186		
		11.3.3	Experimental Constraints for the Gas Exchange			
			Model for Carbon Dioxide	189		
		11.3.4	Experimental Design and Test Signal Selection	190		
	11.4	An Inh	omogeneous Lung Model with Tidal Ventilation	194		
		11.4.1	Identifiability Analysis of the Inhomogeneous			
			Lung Model	196		
	11.5	Applica	ations of Respiratory Gas-Exchange Models	196		
	11.6	Quality	V Issues in Gas-Exchange Modelling	198		
	Refer	ences		199		
12	Case Study: Modelling of Elements of the Neuromuscular					
	Syste	ms Invo	lved in Regulation of Posture and Control			
	of Me	ovement	- -	203		
	12.1	Introdu	ction	203		
	12.2 Mathematical and Computer-Based Modelling		natical and Computer-Based Modelling			
		of the S	System	204		
	12.3	of the S The Ph	System	204 205		
	12.3 12.4	of the S The Ph Models	System	204 205 207		
	12.3 12.4	of the S The Ph Models 12.4.1	System	204 205 207		
	12.3 12.4	of the S The Ph Models 12.4.1	System	204 205 207 208		
	12.3 12.4	of the S The Ph Models 12.4.1	System	204 205 207 208 211		
	12.3 12.4	of the S The Ph Models 12.4.1 12.4.2 12.4.2	System	204 205 207 208 211 215		
	12.3 12.4	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell	System	204 205 207 208 211 215 215		
	12.3 12.4 12.5	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1	System ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems s of Skeletal Muscle Development of an Experimental Model of Skeletal Muscle Testing and Validation of the Muscle Model Testing and Validation of the Muscle Model Testing and Validation of the Muscle Model ing of Other Elements of the Neuromuscular System Modelling of Signal Transmission Pathways	204 205 207 208 211 215 215 215		
	12.3 12.4 12.5	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1 12.5.2	System ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems s of Skeletal Muscle Development of an Experimental Model of Skeletal Muscle Testing and Validation of the Muscle Model Testing and Validation of the Muscle Model Testing and Validation of the Muscle Model ing of Other Elements of the Neuromuscular System Modelling of Signal Transmission Pathways	204 205 207 208 211 215 215 215 215		
	12.3 12.4 12.5	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1 12.5.2 12.5.2	System	204 205 207 208 211 215 215 215 218 223		
	12.3 12.4 12.5	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1 12.5.2 12.5.3	System	204 205 207 208 211 215 215 215 218 223		
	12.3 12.4 12.5 12.6	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1 12.5.2 12.5.3 Models of Simu	System ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems sof Skeletal Muscle Development of an Experimental Model of Skeletal Muscle of Skeletal Muscle sof Skeletal Muscle Testing and Validation of the Muscle Model sof Skeletal Applications of the Muscle Model sof Skeletal ing of Other Elements of the Neuromuscular System sof Modelling of Signal Transmission Pathways Modelling of Sensory Receptors sof the Neuromuscular Control System and the Role ulation in the Testing of Hungchases sof Hungchases	204 205 207 208 211 215 215 215 218 223		
	12.3 12.4 12.5 12.6	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1 12.5.2 12.5.3 Models of Simu	System ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems sof Skeletal Muscle Development of an Experimental Model of Skeletal Muscle of Skeletal Muscle Testing and Validation of the Muscle Model Testing and Validation of the Muscle Model model ing of Other Elements of the Neuromuscular System Modelling of Signal Transmission Pathways Modelling of Sensory Receptors The Testing of Models of Sensory Receptors so of the Neuromuscular Control System and the Role alation in the Testing of Hypotheses	204 205 207 208 211 215 215 215 218 223 224		
	12.3 12.4 12.5 12.6	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1 12.5.2 12.5.3 Models of Simu 12.6.1	System ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems s of Skeletal Muscle Development of an Experimental Model of Skeletal Muscle Testing and Validation of the Muscle Model Testing and Validation of the Muscle Model Applications of the Muscle Model ing of Other Elements of the Neuromuscular System Modelling of Signal Transmission Pathways Modelling of Sensory Receptors The Testing of Models of Sensory Receptors s of the Neuromuscular Control System and the Role alation in the Testing of Hypotheses Testing of Models of the Neuromuscular Control System	204 205 207 208 211 215 215 215 215 218 223 224		
	12.3 12.4 12.5 12.6	of the S The Ph Models 12.4.1 12.4.2 12.4.3 Modell 12.5.1 12.5.2 12.5.3 Models of Simu 12.6.1	System ysiology of Neuromuscular Systems ysiology of Neuromuscular Systems psiology of Neuromuscular Systems s of Skeletal Muscle Development of an Experimental Model of Skeletal Muscle Testing and Validation of the Muscle Model Testing and Validation of the Muscle Model Applications of the Muscle Model ing of Other Elements of the Neuromuscular System Modelling of Signal Transmission Pathways Modelling of Sensory Receptors The Testing of Models of Sensory Receptors s of the Neuromuscular Control System and the Role ulation in the Testing of Hypotheses Testing of Models of the Neuromuscular Control System	204 205 207 208 211 215 215 215 218 223 224 227 228		

13	Furth	ner Discussion	233
	13.1	Principles and Practices of Model Testing: An Overview	233
	13.2	Strategic Issues in Modelling and Simulation	
		and Current Trends in Model Verification, Validation	
		and Accreditation	236
	13.3	Research and Development Opportunities in the Field	
		of Model Quality Assessment	240
	13.4	Educational Issues	241
	13.5	Final Remarks	242
	Refer	ences	243
Ind	ex		245

Abbreviations

ADC	Analogue to digital converter
AGARD	Advisory Group on Aerospace Research and Development (NATO)
AIAA	American Institute of Aeronautics and Astronautics
ANL	Argonne National Laboratory (US)
ASCI	Accelerated Strategic Computing Initiative
ASME	American Society of Mechanical Engineers
BIM	Building Infrastructure Management
CAD	Computer-aided design
CFD	Computational fluid dynamics
DAC	Digital to analogue converter
DAE	Differential algebraic equation
DLR	Deutsches Zentrum fűr Luft- und Raumfahrt (German Aerospace
	Centre)
DMSO	Defense Modeling and Simulation Office (US)
DSB	Defense Science Board (US)
ESA	European Space Agency
FMI	Functional Mock-up Interface
FNS	Functional neuromuscular stimulation
FRAC	Frequency response assurance criterion
FRF	Frequency response function
GA	Genetic algorithm
GP	Gaussian process
GP	Genetic programming
ISPOR	International Society for Pharmacoeconomics and Outcomes Research
MC/DC	Modified condition/decision coverage
M&S	Modelling and simulation
M&SCO	Modeling and Simulation Coordination Office (US)
NATO	North Atlantic Treaty Organisation
NSHEB	North of Scotland Hydro-Electric Board
ODE	Ordinary differential equation

ONR	Office of Naval Research (US)
PDE	Partial differential equation
PTB	Project test bed
S3D	Ship-Smart System Design
SA	Simulated annealing
SCS	Society for Computer Simulation
SMDM	Society for Medical Decision Making
SSD	Smart-ship design
TIC	Theil's inequality coefficient
V&V	Verification and validation
VV&A	Verification, validation and accreditation
VTB	Virtual test bed

Chapter 1 An Introduction to Simulation Models and the Modelling Process

1.1 Objectives in Mathematical Modelling and Computer Simulation

Mathematical modelling and computer simulation methods are powerful tools and have applications in many areas of science, engineering, medicine, economics, business and the social sciences. It is clearly possible to describe any real system in different ways and the number of possible models that can be used in any specific case is infinite. In practice, we have to find ways of assessing the suitability or otherwise of a model for a proposed application and for comparing different models in terms of objective measures or, in many cases, through procedures that are more subjective. This book discusses issues of model testing and evaluation, both for engineering applications and for system modelling in the biological sciences. Four case studies are included, two of which are from engineering and two from physiology. The emphasis throughout is primarily on dynamic models that involve variables that are continuous functions of time. The methods being discussed thus relate mainly to models implemented using continuous system simulation tools.

It is important to note, from the outset, that there is an important difference between ways in which mathematical modelling and computer simulation are used by engineers and the ways in which these techniques are employed for broader scientific investigations where the objectives are often very different from those in engineering. Probably the most important factor relates to the uncertainties in our understanding of the real system represented by the model and the extent to which there are unknown, or incompletely understood, elements. Although engineering systems involve uncertainties and models of those systems have limitations, they are often relatively well understood in terms of their structure. Within that field, models can be very useful in specific applications and are most often developed to help in the design of new engineering products, or to allow testing and analysis of an existing engineering product or system. Most engineering systems are thus well understood in terms of their structure and are often described as "closed".

In contrast to engineering systems, natural systems arising in scientific fields such as physiology and the environmental sciences often involve models that are not closed. Information about the real system represented by the model is incomplete or has been derived through processes involving fairly drastic simplifications and approximations. The system boundaries are often ill-defined and involve major uncertainties. In science, a model is most often a stepping-stone within a research project which is aimed primarily at providing a better understanding of a natural phenomenon and models may be especially helpful in the design of experiments for the testing of hypotheses. Model development and computer simulation techniques, thus become a central and natural part of the scientific method. It is interesting to note that in clinical medicine we find some applications of modelling and simulation that show quite strong similarities to some types of model-based investigations in engineering, while other medical applications may involve problems which display all the uncertainties and the open-ended nature of investigations in pure science.

In science, observations made of the behaviour of a real system may often be explained in a simple and concise way using a mathematical model or an associated computer-based simulation. More quantitatively, a model may also be used to provide an indirect estimate of something that is difficult to measure directly. Models and the associated computer simulations may be of assistance in making predictions or decisions, such as those relating to climate change, or weather forecasting, or estimates of future changes in air or water quality. They may also have an explanatory role and may be developed as part of an attempt to bring together all the available information about some natural system in a convenient and concise form of description that can be accessed by researchers in different groups around the world.

As with scientific applications, models in engineering may also be used to describe, analyse, explain or simply document a complex system. However, a more important type of application involves the use of these techniques to support the design process and prototype development, or to assist in decision-making processes. Models are often vital for tackling the trade-offs within the design process and properly tested models and computer simulations now provide evidence that is routinely used to establish a basis for certification of the performance, safety and reliability of safety-critical and high-value systems. They provide a way of supplementing the testing of prototype systems and can allow investigation of performance limitations that would not be permitted in more direct ways for reasons of safety or the risk of damage to expensive hardware. Proven models can reduce engineering development times and costs in a significant way and also provide a basis for some techniques of computer-based control, and for more specialised applications such as schemes for automatic fault detection and fault alleviation. Such models are also valuable for the development of real-time simulators that are used routinely for training of operators. Without simulators, risks associated with use of the real hardware would make it impossible to expose operators to training scenarios involving major system problems. A simple example of this could be a pilot being trained to deal with an engine failure or a control surface actuator failure in an aircraft in flight. Other examples of similar safety-critical applications are found in the training of operators for off-shore platforms serving the oil and gas industry, in nuclear power generation and in the control of electricity supply networks.

From all of the above discussion, it is clear that, because of the important role of simulation and modelling techniques in many different fields, the adoption of proper procedures for testing models and computer simulations prior to their routine application is very important. The significance of testing is obvious for engineering design, for training simulator development or for simulators on which different management and operational strategies can be investigated. The testing of models is also critically important in scientific investigations since any publication of results that depend on a simulation model should include details of the processes used for assessing the model's fitness-for-purpose. Publications relating to models and the associated simulation software must provide proper "transparency" so that the reader can extract all the information required to fully understand the model and how it has been tested. Ideally the reader should be able, in principle at least, to assemble the model from the information provide and reproduce all the published findings.

1.2 Requirements Definition and Conceptual Modelling

One key aspect of the model development process is the requirements definition. This starts from basic statements of the purpose of the model, together with statements about its performance, cost and timescale. It ends with a detailed set of specifications and performance targets for the model. Defining the precise purpose of a model often follows on from a functional statement relating to the project for which the model is required and the deliverables from that project. The specification of model fidelity must always be related to the broader performance requirements of the planned application.

Within engineering, a distinction may be made between what have been termed "market pull" projects (perhaps involving design and development of a specific product to meet given performance requirements in a specific period of time) and "technology push" projects intended to assess new areas of technology (such as a new form of control scheme) and reach conclusions about their likely future importance and potential value [1]. In the case of "market pull" projects there is usually a clear problem statement that can be used in the requirements definition for the associated simulation model. With "technology push" projects, on the other hand, the requirements definition for models needed in the investigation may be less precise initially but should always be chosen to be representative of problems to which the new technology could be applied. With technology-push projects a range of different models having distinctly different characteristics in terms of their

structure, order, nonlinearity etc. might be needed to allow firm conclusions to be reached about the potential value of the new ideas.

Examples of major "market pull" projects in which modelling failures or inadequacies have led to significant extra costs or to late delivery are well known. For instance, in naval construction in the USA the average over-cost of new ship classes is reported as being of the order of 30 % and it is believed that a significant reason for this is that designs have been released to production prematurely [2]. It has also been alleged that most of the extra costs could have been predicted at the design stage if the systems had been modelled more comprehensively. These ideas form a central part of the reasoning behind the development by the US Office for Naval Research (ONR) of the Ship-Smart System Design (SSD) tool where it has been recommended, in a rather revolutionary set of proposals, that the system model should become the system specification [3].

Although not all projects in all areas of application, even within engineering, can fit within the framework being suggested by ONR, it is obvious that whatever the area of application clear definitions of model requirements are of critical importance. This applies equally to "technology push" projects and to work within other disciplines such as the physical, biological and earth sciences. It should be noted that, in practice, model specifications may change and evolve during a project due to the understanding that is built up during the work, even if the formal requirements remain the same throughout.

Following requirements definition, an early stage of most projects involves the assembling of all available information about the structure and function of the system or the formation of hypotheses for cases involving much uncertainty, as is the case in modelling some physiological systems. The dominant phenomena within the system to be modelled must first be identified and described, initially in terms of words. This could involve energy conversion and storage processes, or material transfer and storage within distinct compartments. Appropriate simplifying assumptions can then be applied to create an initial "conceptual" model. The development of the conceptual model is a highly creative task that often has intuitive elements. The model must include all relevant available knowledge about the important phenomena involved to allow a possible model structure to be defined, together with parameters of the system and important variables. It is particularly important to identify the variables that have measurable counterparts within the real hardware as these are potentially important for model validation.

Essentially, a conceptual model is a collection of statements, assumptions, relationships and data that describe the reality of interest. From this conceptual type of description a mathematical model can eventually be constructed and information useful in the design of experiments to test that model can be derived [4]. Often a top-down approach is adopted, where a relatively coarse type of description is defined initially, with details being added at a later stage. However, there are usually also elements of bottom-up thinking where existing sub-models are introduced within the structure that has been defined in a top-down fashion at the start.

This initial process of conceptual modelling is followed by the abstraction of the information contained within the qualitative description to provide a more formal representation, usually involving the use of equations or graphical block diagram elements. The choice, in this respect, may depend on the modelling tools and computing environment chosen for the work. This mathematical model not only involves equations but also boundary values, initial conditions and data needed to describe the conceptual model in quantitative terms [4]. That can provide information about key parameter sensitivities and inter-dependencies which may be important for design decisions and for performance optimisation.

1.3 Issues of Model Quality

Since a model is only an abstraction of the system it represents, perfect accuracy is impossible. This inevitably raises important philosophical questions but, in all fields in which modelling and simulation techniques are used, the key issue is one of determining the level of model fidelity needed for the intended application. Models also need to be transparent so that all who make use of a model can have some understanding of how it is organised. An inappropriate model is less than useless and, in engineering applications, may delay the project and lead to cost escalation. In scientific research projects, the use of incorrect or poorly understood models may lead investigators in totally the wrong direction. In general, whatever the type of application, modelling errors should be reduced to defined levels for specified operating regions for the system. Information about these modelling errors and a "neighbourhood of validity" must be readily available to users along with all the other information about the model that provide the required overall transparency.

While reducing modelling errors is very important, a balance should also be sought between overall accuracy and other factors. These include development time, solution speed and the cost of developing the model in relation to the expected benefits. In any type of application, the level of detail within a model is linked to its purpose. As models are made more detailed, they inevitably become more complex but model complexity should never be confused with model quality and a simple description can often be better, in terms of quality measures, than a more complex one. Developing a model requires careful examination of information about the real system and consideration of how the model is to be used. In general terms, when modelling a complex dynamic system, it is advisable to move in a stepwise fashion from a well-understood area of operation, such as a steady-state condition, towards situations where knowledge is more limited. Inconsistencies or gaps in the available knowledge can then be found. These may require further experimental work or the testing of an engineering prototype and this process may lead sometimes to a reconsideration of requirements. The outcome of the model assessment process should be a statement of the quantified level of agreement between experimental data and model prediction, as well as information about the predictive accuracy of the model [4].

Tested models allow virtual prototypes to be created before any hardware prototype is available. This provides a way of identifying necessary design alterations at an early stage and, perhaps, of avoiding expensive changes later on. Once real prototypes become available more complete and rigorous processes of testing and model validation become possible, as discussed in Chap. 2.

1.4 Model Re-use

In terms of the overall efficiency of the modelling process, re-use of model components is important and some software tools for modelling and simulation now offer well-documented libraries of re-usable sub-models that are based on the previous experience of many different users. Successful re-use requires sound principles of model management and this is especially important for applications involving large teams of developers, especially when these include multidisciplinary groups and geographically dispersed teams.

In the field of medical decision making some health care models are intended to be "general" in the sense that they can provide a basis for a number of investigations. Other models are built for a single application and are not intended to be re-used but may, in fact, be modified and extended at a later date so that they can be applied to new situations. This division between "general" and "specific" models is also likely to apply in other fields. For a "multi-application" model, with more general applicability, transparency is clearly a priority and the documentation must therefore be of the highest quality. In such cases validation is an on-going process and the model is likely to have to be modified and updated as science advances. In such situations, retaining full documentation for each historical version of a model is important. For a model intended for a single application, issues of transparency and model validation are still vitally important because information about the model has to be fully reported when results from the research are published. Also, a "single-application" model may well be picked up again at some future date by a new user who is interested in a new project with slightly different objectives and may be interested in the possibility of re-using some specific feature of that earlier model.

1.4.1 Model Libraries

A library of models or sub-models, for use in a particular application area, needs not only to be designed to meet current requirements but also to satisfy possible needs in the future [5]. Sub-models should therefore be designed as building blocks for a range of applications rather than specifically for one project. This means that verification and validation processes should be applied, first of all, at the sub-model level and should be subjected to testing over a range of conditions before being accepted, documented and made available for wider use.

One of the most important reasons for model re-use is that it can reduce the time required for the development of new models. A library also allows the investigator to make an informed decision about the sub-model that best meets their needs. This might involve selecting a specific sub-model from a number of representations involving different levels of detail. Within a library, it is useful to establish a taxonomy of models [6], which incorporates generic model classes and sub-classes. This becomes more and more important as the number of models increases. Ideally the library should also allow the modeller to cross from one energy domain to another. As an example, this feature might allow a design engineer to move easily from consideration of a hydraulic actuator for a specific application to examining the possible use of an electrical actuator for the same task.

Some modern object-oriented simulation software environments, such as Modelica® [7], provide standard model libraries and allow new libraries to be developed. Other packages can be extended with tools for physical modelling in various domains. An example of this is MATLAB®/Simulink® [8] which includes some standard library sub-models and, through SimscapeTM [9] there are additional standard libraries involving sub-models for fields such as mechanics, hydraulics, electronics, mechanical transmission systems and electrical power systems. Using the SimscapeTM language, which is based on MATLAB® [8], new sub-models can be created together with equivalent Simulink® blocks, for components and sub-systems that are not included in existing libraries.

In projects which involve several teams working together, team members may wish to use different tools and languages when building their models of different sub-systems. Sub-models from different software environments may then have to be brought together within some larger model. One example of this is the Virtual Test Bed (VTB) [10] which is an environment that facilitates integration of sub-models developed using other widely-used tools [11], such as MATLAB®/ Simulink® [8], Modelica® or VHDL-AMS [12]. This has obvious significance in terms of verification processes and inevitably requires further checks beyond those performed on the original sub-model.

1.4.2 Generic Models

"Generic" models extend the ideas associated with model libraries. A generic simulation model can be applied to a number of different projects without significant internal reorganisation. The essential requirements of a generic description must be identified first and a suitable framework established that offers sufficient flexibility for a number of different sets of objectives. The main benefit of adopting a generic approach is that it may lead to savings in the development of a whole series of models for different projects, compared with the traditional approach involving the separate development of a new model to suit each application.

Benefits may also arise because a generic model requires more rigour in terms of model validation, together with better documentation. However the advantages are only realised if the generic model, once developed, is used for a range of different projects and the potential range of applications requires careful consideration prior to any decision to embark on the development of a model of this kind. Issues arising in the testing and validation of library sub-models and generic models are discussed in Chap. 7.

Examples of the generic approach can be found at present in several application areas, including communication systems (e.g. [13]), automotive engineering (e.g., [14]), electro-optic systems (e.g. [15]) and the planning of critical care resource requirements [16]. A good example is the European Space Agency (ESA) Generic Project Test Bed (PTB) which involves re-usable simulator architectures for space-craft design [17]. The generic structure includes ground-station models as well as spacecraft sub-systems, together with models relating to the environment. It is important to note that the PTB allows for real-time simulation and hardware-in-the-loop operation and this is a feature that can also be found in some other examples of the generic approach.

1.5 Classes of Model

Many dynamic models used in science and engineering involve variables that are continuous functions of time, such as position, velocity, acceleration, temperature or pressure. Models based on these continuous-variable descriptions may involve ordinary or partial differential equations or differential-algebraic equations. This is the main class of model considered in this book and within this general class there can be many variations in terms of the model structure.

A second class of model that can be important, not only in science and engineering but also in other areas, such as business, planning and operations research, involves discrete-event descriptions. In such models all the variables remain constant between events that mark changes in the model. These changes take place at discrete time instants, either periodically or in a random fashion. Simple examples arise in applications which involve queues, such as in modelling a shop or bank to establish how many tills need to be provided to ensure that customer waiting times are acceptable. A digital computer used for real-time control is another example of a discrete system involving periodic changes. In this case, a continuous variable may be sampled periodically using an analogue-to-digital converter. Calculations carried out using the discrete values obtained from the converter are then changed back into continuous variable form using a digital-to-analogue converter. In modelling this type of component within some larger engineering system we cannot use differential equations because of the discrete nature of the events within the digital processor and an approach involving a discrete model (based on differenceequations instead of differential equations) is more appropriate. However, hybrid models, involving representations that are mainly continuous but do involve some discrete-event elements are becoming increasingly common.

1.5.1 Models Involving Continuous Variables

Within the class of continuous variable dynamic models we can distinguish between models of data and physically-based models of systems. A model of data involves a description fitted to measured responses, usually from a real physical system, leading to a model that expresses an observed relationship between two or more variables. It consists of mathematical functions that may have no direct link to recognisable elements of the real system. Models of this kind are important in fields such as control engineering where input-output descriptions, such as transfer functions, may be used. Often these models may be derived directly from measurements and are often termed "black box" models. They may provide a useful starting point for engineering design but incorporate limited information about internal processes. If they are derived entirely from experimental data their validity is restricted to the conditions that applied in those experiments. Physically-based models, on the other hand, are developed using established scientific principles, such as basic laws and principles from physics, chemistry and biology. The models and sub-models being considered in this book thus range from completely transparent descriptions based on physical principles, through intermediate "grey-box" descriptions, to the entirely empirical black-box form of experimentally-derived model.

Another important distinction is between linear and nonlinear models. Linear models are attractive because they are open to analysis and can be incorporated conveniently into design procedures. However, linear descriptions may be incapable of capturing aspects of the behaviour of the real physical system and issues of nonlinearity should be considered at an early stage in modelling. Assumptions of linearity should not be made without justification and the range of linear operation of the system always needs to be evaluated when a linear description is used. Dangers arise if the model is chosen for reasons of mathematical convenience and the developer fails to recognise properly the complex realities of the real world situation.

A time-invariant description is one in which the performance of the system being modelled is independent of the times at which observations are made. As with questions of linearity, time invariance needs to be demonstrated rather than assumed. Models that are linear and time invariant receive particular attention in many engineering textbooks dealing with topics such as electrical circuit theory, signal processing, dynamics and automatic control. Many systems have properties that allow them to be described by linear time-invariant models for some operating conditions and such models are very attractive because they can be analysed using simple linear methods of mathematics, such as Laplace transform techniques. Although nonlinear and time-varying dynamic models are more general, they are harder to deal with using mathematical methods and numerical and computer simulation techniques have therefore become very important for such models. Simulation thus offers valuable insight for problems that would otherwise be intractable.

1.5.1.1 Models Based on Ordinary Differential Equations and Differential Algebraic Equations

Mathematical descriptions based entirely on linear or nonlinear ordinary differential equations (ODEs) form a particularly important class of model. A broader class of model involves differential algebraic equations (DAEs) which include algebraic relations in addition to the ODEs. In both cases all the quantities in these models are simply functions of time and do not change with spatial coordinates. These are known as lumped-parameter descriptions and are important for many situations involving, for example, mechanical systems, electrical networks and compartmental systems arising in the modelling of chemical processes or physiological systems.

1.5.1.2 Models Based on Partial Differential Equations

Models based on partial differential equations (PDEs) are important for modelling systems that involve quantities that are physically distributed and thus depend on spatial coordinates as well as time. One example could relate to the temperature distributions in a material where, in a lumped representation, this would be modelled in an approximate way by using a mean value of temperature over some region. As well as containing derivatives of variables with respect to time, a model based on PDEs would also contain derivatives with respect to spatial variables. In general terms, lumped models based on ODEs can be viewed as approximations of distributed parameter descriptions based on PDEs.

A simple example of a PDE model is the heat flow equation:

$$\frac{\partial u}{\partial t} - c \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = f \tag{1.1}$$

where the variable u represents the temperature at the position (x, y) in the material. The variable u depends both on time, t, and the spatial position defined by the variables x and y. The quantities c and f are constant parameters in the simplest form of the heat equation but could be functions of the spatial coordinates x and y.

Distributed parameter models are discretised in order to allow conventional simulation tools to be applied. This involves all partial derivatives being expanded and approximated by sets of algebraic equations and differential equations at discrete points to give a set of DAEs that can be handled using standard tools. Techniques commonly used to discretise partial differential equations for simulation include finite element methods, finite difference methods and the method of lines, analytical methods, the integral approximation method, Padé approximation methods, the Ritz method and Galerkin's method. Further details of these techniques may be found in texts dealing specifically with the solution of partial differential equations (see, e.g. [18]). Some simulation environments, such as MapleSimTM [19] include tools that can be used to discretise PDEs and automatically generate components that can be used for simulation. For example, recent developments [20] have provided a method of incorporating PDEs within a Modelica model by using the Functional Mock-up Interface (FMI) [21] of Modelica to import a PDE solver from the HiFlow3 multi-purpose finite element library written in C++ [22]. With further extensions it is believed that this could provide a relatively simple approach which allows re-use of existing software which is known to be efficient and to have been fully verified [20].

In some specific cases it is possible to use analytical techniques to reduce a description based on partial differential equations to a model involving a lumped approximation. Whether or not it is appropriate to approach the model development in this way depends on the application for which the model is being developed. One example of this is the reduction of a distributed parameter model to a lumped representation involving a pure time delay.

A useful set of papers on the modelling, analysis and control of distributed parameter systems may be found in a special issue of the journal *Mathematical and Computer Modelling of Dynamical Systems* published in 2011 with guest editors Kurt Schlacher and Markus Schöberl of the Johannes Kepler University of Linz [23]. The papers in that special issue relate both to theoretical problems concerning the development of distributed parameter models and to a number of applications, including the modelling of flexible structures for sub-sea applications [24].

1.5.2 Discrete-Event and Hybrid Models

In discrete-event models changes of the values of system variables are assumed to occur instantaneously and in a discontinuous fashion at specific instants of time. Such a representation is clearly approximate since real physical variables cannot change instantaneously and the idea behind discrete-event models is to make the model more tractable and to speed-up the simulation significantly. The variables of a discrete-event model change value at specific points in time and these are termed events. Values of variables remain constant between events.

One important example of discrete-event modelling concerns the dynamics of manufacturing systems. Problems in that field can be especially challenging when they relate to the overall dynamics of a network of interacting manufacturing systems and the associated supply chains. In most practical applications of this kind there are a number of well-defined steps associated with fabrication, testing, assembling and packaging. In all kinds of manufacturing the total flow time is influenced by many different factors, such as the processing time at each stage of