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William L. Oberkampf and Christopher J. Roy
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VERIFICATION AND VALIDATION IN SCIENTIFIC COMPUTING

Advances in scientific computing have made modeling and simulation an important part of the decision-making process in engineering, science, and public policy. This book provides a comprehensive and systematic development of the basic concepts, principles, and procedures for verification and validation of models and simulations. The emphasis is placed on models that are described by partial differential and integral equations and the simulations that result from their numerical solution. The methods described can be applied to a wide range of technical fields, such as the physical sciences, engineering, and technology, as well as to a wide range of applications in industry, environmental regulations and safety, product and plant safety, financial investing, and governmental regulations.

This book will be genuinely welcomed by researchers, practitioners, and decision-makers in a broad range of fields who seek to improve the credibility and reliability of simulation results. It will also be appropriate for either university courses or independent study.

WILLIAM L. OBERKAMPF has 39 years of experience in research and development in fluid dynamics, heat transfer, flight dynamics, and solid mechanics. He has worked in both computational and experimental areas, and taught 30 short courses in the field of verification and validation. He recently retired as a Distinguished Member of the Technical Staff at Sandia National Laboratories.

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To our wives, Sandra and Rachel

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The color plates will be found between pages 370 and 371.

Preface

Modeling and simulation are used in a myriad of ways in business and government. The range covers science, engineering and technology, industry, environmental regulations and safety, product and plant safety, financial investing, design of military systems, governmental planning, and many more. In all of these activities models are built that are mental constructs of how we believe the activity functions and how it is influenced by events or surroundings. All models are abstractions of the real activity that are based on many different types of approximation. These models are then programmed for execution on a digital computer, and the computer produces a simulation result. The simulation result may have high fidelity to the actual activity of interest, or it may be complete nonsense. The question is: how can we tell which is which? This book deals with various technical and procedural tools that can be used to assess the fidelity of modeling and simulation aspects of scientific computing. Our focus is on physical processes and systems in a broad range of the natural sciences and engineering.

The tools discussed here are primarily focused on mathematical models that are represented by differential and/or integral equations. Many of these mathematical models occur in physics, chemistry, astronomy, Earth sciences, and engineering, but they also occur in other fields of modeling and simulation. The topics addressed in this book are all related to the principles involved in assessing the credibility of the models and the simulation results. We do not deal with the specific details of modeling the physical process or system of interest, but with assessment procedures relating to the fidelity of the models and simulations. These procedures are typically described by the terms *verification* and *validation*.

We present the state of the art in verification and validation of mathematical models and scientific computing simulations. Although we will discuss the terminology in detail, *verification* can simply be described as "solving the equations right" and *validation* as "solving the right equations." Verification and validation (V&V) are built on the concept of quantitative accuracy assessment. V&V do not answer the entire question of simulation credibility, but they are key contributors. V&V could be described as the processes that provide evidence of the correctness and/or accuracy of computational results. To measure correctness, one must have accurate benchmarks or reference values with which to compare. However, the majority of simulations of complex processes do not have a computable or measurable reference value. For these situations we must rely on numerical error estimation and estimation of the effects of all of the contributors to uncertainty in system responses. In verification, the primary benchmarks are highly accurate solutions to specific, although limited, mathematical models. In validation, the benchmarks are high-quality experimental measurements of system response quantities of interest. These experimental measurements, and the detailed information of the system being tested, should also have carefully estimated uncertainty in all of the quantities that are needed to perform a simulation of the experiment.

Mathematical models are built and programmed into software for the purpose of making predictions of system responses for cases where we do not have experimental data. We refer to this step as *prediction*. Since prediction is the usual goal of modeling and simulation, we discuss how accuracy assessment results from V&V activities enter into prediction uncertainty. We discuss methods for including the estimated numerical errors from the solution of the differential and/or integral equations into the prediction result. We review methods dealing with model input uncertainty and we present one approach for including estimated model uncertainty into the prediction result. The topic of how to incorporate the outcomes of V&V processes into prediction uncertainty is an active area of current research.

Because the field of V&V for models and simulations is in the early development stage, this book does not simply provide a prescriptive list of steps to be followed. The procedures and techniques presented will apply in the majority of cases, but there remain many open research issues. For example, there are times where we point out that some procedures may not be reliable, may simply not work, or may yield misleading results.

As the impact of modeling and simulation has rapidly increased during the last two decades, the interest in V&V has also increased. Although various techniques and procedures have been developed in V&V, the philosophical foundation of the field is *skepticism*. Stated differently, if the evidence for computer code correctness, numerical error estimation, and model accuracy assessment are not presented as part of a prediction, then the V&V perspective presumes these activities were not done and the results should be questioned. We feel this is the appropriate counter balance to commonly unsubstantiated claims of accuracy made by modeling and simulation. As humankind steadily moves from decision making primarily based on system testing to decision making based more heavily on modeling and simulation, increased prudence and caution are in order.

Acknowledgments

Although only two names appear on the cover of this book, we recognize that if other people had not been there for us, and many others had not helped, this book would have never been written. These people provided training and guidance, created opportunities, gave advice and encouragement, corrected us when we were wrong, and showed the way to improved understanding of the subject. Although there were many pivotal individuals early in our lives, here we only mention those who have contributed during the last decade when the idea for this book first came to mind.

Timothy Trucano, Frederic Blottner, Patrick Roache, Dominique Pelletier, Daniel Aeschlimam, and Luís Eça have been critical in generously providing technical insights for many years. We have benefited from their deep knowledge of verification and validation, as well as a number of other fields. Jon Helton and Scott Ferson have guided our way to an understanding of uncertainty quantification and how it is used in risk-informed decision making. They have also provided key ideas concerning how to connect quantitative validation results with uncertainty estimates in model predictions. Without these people entering our technical lives, we would not be where we are today in our understanding of the field.

Martin Pilch created opportunities and provided long-term funding support at Sandia National Laboratories, without which we would not have been able to help advance the state of the art in V&V. He, along with Paul Hommert, Walter Rutledge, and Basil Hassan at Sandia, understood that V&V and uncertainty quantification were critical to building credibility and confidence in modeling and simulation. They all recognized that both technical advancements and changes in the culture of people and organizations were needed so that more reliable and understandable information could be provided to project managers and decision makers.

Many colleagues provided technical and conceptual ideas, as well as help in working through analyses. Although we cannot list them all, we must mention Mathew Barone, Robert Croll, Sharon DeLand, Kathleen Diegert, Ravi Duggirala, John Henfling, Harold Iuzzolino, Jay Johnson, Cliff Joslyn, David Larson, Mary McWherter-Payne, Brian Rutherford, Gary Don Seidel, Kari Sentz, James Stewart, Laura Swiler, and Roger Tate. We have benefited from the outstanding technical editing support through the years from Rhonda Reinert and Cynthia Gruver. Help from students Dylan Wood, S. Pavan Veluri, and John Janeski in computations for examples and/or presentation of graphical results was vital.

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We were blessed with encouragement and patience from our wives, Sandra and Rachel. They tolerated our long hours of work on this book for longer than we deserved.