

## Uncertainty Quantification In Computational Fluid Dynamics Lecture Notes In Computational Science And Engineering

*Uncertainty Quantification in Multiscale Materials Modeling provides a complete overview of uncertainty quantification (UQ) in computational materials science. It provides practical tools and methods along with examples of their application to problems in materials modeling. UQ methods are applied to various multiscale models ranging from the nanoscale to macroscale. This book presents a thorough synthesis of the state-of-the-art in UQ methods for materials modeling, including Bayesian inference, surrogate modeling, random fields, interval analysis, and sensitivity analysis, providing insight into the unique characteristics of models framed at each scale, as well as common issues in modeling across scales.*

*This book proposes the formulation of an efficient methodology that estimates energy system uncertainty and predicts Remaining Useful Life (RUL) accurately with significantly reduced RUL prediction uncertainty. Renewable and non-renewable sources of energy are being used to supply the demands of societies worldwide. These sources are mainly thermo-chemo-electro-mechanical systems that are subject to uncertainty in future loading conditions, material properties, process noise, and other design parameters. It book informs the reader of existing and new ideas that will be implemented in RUL prediction of energy systems in the future. The book provides case studies, illustrations, graphs, and charts. Its chapters consider engineering, reliability, prognostics and health management, probabilistic multibody dynamical analysis, peridynamic and finite-element modelling, computer science, and mathematics.*

*Bringing together the world's leading researchers and practitioners of computational mechanics, these new volumes meet and build on the eight key challenges for research and development in computational mechanics. Researchers have recently identified eight critical research tasks facing the field of computational mechanics. These tasks have come about because it appears possible to reach a new level of mathematical modelling and numerical solution that will lead to a much deeper understanding of nature and to great improvements in engineering design. The eight tasks are: The automatic solution of mathematical models Effective numerical schemes for fluid flows The development of an effective mesh-free numerical solution method The development of numerical procedures for multiphysics problems The development of numerical procedures for multiscale problems The modelling of uncertainties The analysis of complete life cycles of systems Education - teaching sound engineering and scientific judgement Readers of Computational Fluid and Solid Mechanics 2003 will be able to apply the combined experience of many of the world's leading researchers to their own research needs. Those in academic environments will gain a better insight into the needs and constraints of the industries they are involved with; those in industry will gain a competitive advantage by gaining insight into the cutting edge research being carried out by colleagues in academia. Features Bridges the gap between academic researchers and practitioners in industry Outlines the eight main challenges facing Research and Design in Computational mechanics and offers new insights into the shifting the research agenda Provides a vision of how strong, basic and exciting education at university can be harmonized with life-long learning to obtain maximum value from the new powerful tools of analysis*

*Atherosclerotic coronary artery disease continues to negatively impact the lives of millions worldwide. Computational fluid dynamics modeling of coronary blood flow has the potential to help improve clinical outcomes and aid in treatment planning. Significant advancements in coronary blood flow modeling in recent years have opened a wide range of applications such as assessing risk for disease progression or providing a platform for virtual surgery and treatment planning. To encourage the growth of this field and promote adoption of computational results in the clinic, it is crucial that these tools be made as automated as possible so they can be applied to large patient cohorts. In addition, the variability of computational results with respect to uncertainties in the inputs and model must be better understood and systematically quantified. Addressing these concerns is the subject of this thesis. In the first part, a framework for automatically tuning the lumped parameter boundary conditions in simulations of coronary blood flow is developed and demonstrated. Specifying boundary conditions in complex computational models is not a trivial task, especially when the dimensionality of the input space is high and multiple constraints on the outputs need to be satisfied simultaneously. Specifically in the context of patient-specific coronary simulations, clinical data such as the blood pressure, cardiac output, and coronary flow waveforms must be simultaneously satisfied with a large set of input parameters that include lumped resistances, capacitances, and heart model parameters. A typical user can eventually gain expertise to modify the input parameters to satisfy targets, but this manual tuning is time-consuming and not easily reproduced. We thus formulate the automated tuning process as a Bayesian inverse problem in which the model parameters are treated as random variables, and optimal parameters are determined by finding the maximum of the posterior distribution of input parameters. We also perform sensitivity analysis on the input parameters to determine a subset of thirteen parameters that most influence the clinical targets. In the second part, we perform uncertainty quantification on patient-specific simulations of coronary artery bypass graft hemodynamics. Vein graft failure in patients with coronary bypass continues to be a major clinical issue with relatively little knowledge about the mechanisms for failure. Simulations have shown that predicted quantities such as wall shear stress or wall strain can be useful in predicting vein graft failure, but adoption of such results in clinical practice is hindered due to the fact simulations can only produce deterministic results with no range of confidence. Uncertainty quantification provides a framework for quantifying the uncertainty in computational results, and we applied it to assess the variability in computed predictions of time-average wall shear stress and wall strain under uncertainty in the lumped parameter boundary conditions and vessel wall material properties.*

*To achieve this aim efficiently, we develop a novel submodeling strategy for reducing the computational cost of the analysis. We also, for the first time, consider spatial variability in the graft wall material properties by using a random field description. We finally propagate these uncertainties forward using a newly developed multi-resolution approach. The results show that the time-averaged wall shear stress is relatively well estimated with confidence intervals about 35% of the mean value, but the wall strain exhibited significantly more variability due to the large uncertainty in the material properties. In the third part, we perform a comparison of methods for modeling wall deformability in vascular blood flow simulations. Though sometimes neglected, wall deformability can have significant impacts on the computational results, affecting predictions of wall shear stress and precluding calculation of stresses and strains in the vessel wall. There are several methods proposed in the literature for modeling wall deformability, two of the most popular being the Arbitrary Lagrangian Eulerian (ALE) and Couple Momentum Methods (CMM). Although both methods capture the essential characteristics of wall deformability, they can produce different results and computational performance. This provides a rigorous comparison which will aid in the choice of deformable wall model. Additionally, we consider the concept of prestress. Because the geometry for a patient-specific simulation is extracted from medical image data of the *in vivo* cardiovascular system, the vessel walls carry an internal stress which holds the geometry in equilibrium with hemodynamic pressures and viscous stresses. We implement prestress in both ALE and CMM contexts and confirm that it is necessary to avoid over-inflation of the anatomic domain. Although studied mostly within the context of coronary flow simulations, the methods and approaches outlined in this thesis are designed to be generally applicable across other domains in computational modeling, fluid dynamics, and biomechanics. Automated tuning is a general framework for assimilating multiple sources of target data to inform optimal input parameter values, and can broadly be applied in multiscale modeling. The methods for uncertainty quantification can be adapted to assess variability of simulations in other computational fluid mechanics and biomechanics contexts. The results from the wall deformability comparison can also be extended to apply to other contexts including other cardiovascular diseases, respiratory flow, and medical devices. In addition to providing insights into coronary flow simulations, this thesis aims to motivate the importance of tuning, uncertainty quantification, and model comparisons for other cardiovascular simulations and multiscale biological modeling more broadly.*

*Probabilistic Methods for the Quantification of Uncertainty and Error in Computational Fluid Dynamic Simulations*

*Uncertainty Management for Robust Industrial Design in Aeronautics*

*Computational Modelling and Uncertainty Quantification of Blood Flow in the Coronary Arteries*

*Presented at the 1995 ASME/JSME Fluids Engineering and Laser Anemometry Conference and Exhibition, August 13-18, 1995, Hilton Head, South Carolina*

*PIV Uncertainty Methodologies for CFD Code Validation at the MIR Facility*

This book provides an overview of state-of-the-art uncertainty quantification (UQ) methodologies and applications, and covers a wide range of current research, future challenges and applications in various domains, such as aerospace and mechanical applications, structure health and seismic hazard, electromagnetic energy (its impact on systems and humans) and global environmental state change. Written by leading international experts from different fields, the book demonstrates the unifying property of UQ theme that can be profitably adopted to solve problems of different domains. The collection in one place of different methodologies for different applications has the great value of stimulating the cross-fertilization and alleviate the language barrier among areas sharing a common background of mathematical modeling for problem solution. The book is designed for researchers, professionals and graduate students interested in quantitatively assessing the effects of uncertainties in their fields of application. The contents build upon the workshop "Uncertainty Modeling for Engineering Applications" (UMEMA 2017), held in Torino, Italy in November 2017.

"A mixed aleatory (inherent) and epistemic (model-form) uncertainty quantification (UQ) analysis method was applied to a computational fluid dynamics (CFD) modeling problem of synthetic jet actuators. A test case, (Case 3, flow over a hump model with synthetic jet actuator control) from the CFDVAL2004 workshop was selected to apply the Second-Order Probability framework implemented with a stochastic response surface obtained from Quadrature-Based Non-Intrusive Polynomial Chaos (NIPC). Three uncertainty sources were considered: (1) epistemic uncertainty in turbulence model, (2) aleatory uncertainty in free stream velocity and (3) aleatory uncertainty in actuation frequency. Uncertainties in both long-time averaged and phase averaged quantities were quantified using a fourth order polynomial chaos expansion (PCE). Results were compared with experimental data available. A global sensitivity analysis with Sobol indices was utilized to rank the importance of each uncertainty source to the overall output uncertainty. The results indicated that for the long-time averaged separation bubble size, the uncertainty in turbulence model had a dominant contribution, which was also observed in the long-time averaged skin friction coefficients at three selected locations. For long-time averaged pressure coefficient, the contributions from free stream velocity and turbulence model are depending on the locations. The mixed UQ results for phase averaged x-velocity distributions at three selected locations showed that the 95% confidence intervals (CI) could generally envelope the experimental data. The Sobol indices showed that near the wall, the turbulence model had a main influence on the x-velocity, while approaching the main stream, the uncertainty in free stream velocity became a larger contributor. The uncertainty in frequency was found to have a very small contribution to both long-time averaged and phase averaged quantities with the range of variance considered"--Abstract, leaf iii.

This book deals with the application of spectral methods to problems of uncertainty propagation and quantification in model-based computations. It specifically focuses on computational and algorithmic features of these methods which are most useful in dealing with models based on partial differential equations, with special attention to models arising in simulations of fluid flows. Implementations are illustrated through applications to elementary problems, as well as more elaborate examples selected from the authors' interests in incompressible vortex-dominated flows and compressible flows at low Mach numbers. Spectral stochastic methods are probabilistic in nature, and are consequently rooted in the rich mathematical foundation associated with probability and measure spaces. Despite the authors' fascination with this foundation, the discussion only includes those theoretical aspects needed to set the stage for subsequent applications. The book is authored by practitioners, and is primarily intended for researchers or graduate students in computational mathematics, physics, or fluid dynamics. The book assumes familiarity with elementary methods for the numerical solution of time-dependent, partial differential equations; prior experience with spectral methods is naturally helpful though not essential. Full appreciation of elaborate examples in computational fluid dynamics (CFD) would require familiarity with key, and in some cases delicate, features of the associated numerical methods. Besides these shortcomings, our aim is to treat algorithmic and computational aspects of spectral stochastic methods with

details sufficient to address and reconstruct all but those highly elaborate examples.

Within a variety of Computational Fluid Dynamics (CFD) applications, maturity levels can vary significantly depending upon modeling approach and the user's knowledge and skills. Recently, application of CFD techniques for Computational Wind Engineering (CWE) has generated strong interest among wind and structural engineers as a possible substitute for or supplement to wind tunnel experimentation, even though CWE is still in a developmental stage. A necessary step toward advancing CWE simulations in wind and structural engineering applications credible is the development of reliable verification and validation (V&V) procedures. Fundamental factors that determine the degree to which CWE simulations are credible include: (i) the quality of the mathematical modeling of the physics of interest; (ii) the depth of understanding by the users/analysts of the details of the model and the simulation results; (iii) the quality of the verification and validation (V&V) procedures applied to the simulation results, and (iv) the quality of the uncertainty quantification procedure applied to those results. This report deals in detail with the sources of inaccuracy in CFD simulations, and concepts and procedures used in V&V and uncertainty quantification.

Spectral Methods for Uncertainty Quantification

Uncertainty Quantification in Computational Science

Uncertainty Modeling for Engineering Applications

Probabilistic Methods for the Quantification of Uncertainty and Error in Computational Fluid Dynamics Simulations

Quantification of Uncertainty in Computational Fluid Dynamics, 1995

"The primary objective of this study was to develop improved methodologies for efficient and accurate uncertainty quantification with stochastic expansions and apply them to problems in supersonic and hypersonic flows. Methods introduced included approaches for efficient dimension reduction, sensitivity analysis, and sparse approximations. These methods and procedures were demonstrated on multiple stochastic models of hypersonic, planetary entry flows, which included high-fidelity, computational fluid dynamics models of radiative heating on the surface of hypersonic inflatable aerodynamic decelerators during Mars and Titan entry. For these stochastic problems, construction of an accurate surrogate model was achieved with as few as 10% of the number of model evaluations needed to construct a full dimension, total order expansion. Another objective of this work was to introduce methodologies used for further advancement of a quantification of margins and uncertainties framework. First, the use of stochastic expansions was introduced to efficiently quantify the uncertainty in system design performance metrics and performance boundaries. Then, procedures were defined to measure margin and uncertainty metrics for systems subject to multiple types of uncertainty in operating conditions and physical models. To demonstrate the new quantification of margins and uncertainties methodologies, two multi-system, multi-physics stochastic models were investigated: (1) a model for reentry dynamics, control, and convective heating and (2) a model of ground noise prediction of low-boom, supersonic aircraft configurations. Overall the methods and results of this work have outlined many effective approaches to uncertainty quantification of large-scale, high-dimension, aerospace problems containing both epistemic and inherent uncertainty. The methods presented showed significant improvement in the efficiency and accuracy of uncertainty analysis capability when stochastic expansions were used for uncertainty quantification."--Abstract, page iii.

**PUBLIC ABSTRACT:** Computational modeling is of particular interest to science and engineering for the improvement of design and development of products and research of physical phenomena. However, confidence in a computational model must be validated prior to its application through comparison to experimental data. The nuclear power industry has interest in the application of computational modeling to plant design, safety, and development for the increased understanding of heat transfer and fluid dynamics. Fluid dynamics, particularly time-varying phenomena within the reactor core, has a strong effect on heat (energy) transfer and transient accident scenarios of a nuclear power plant. While this work was funded by Idaho National Labs, this research is also applicable to engineering design of heat exchangers. This research began May of 2009. The research within this dissertation demonstrates the validation of various time-varying quantities predicted by computational fluid dynamics models (CFD) with the use of experimental measurements. Several CFD turbulence models are implemented and experimental fluid velocity and pressure data are acquired using non-invasive measurement techniques for flow through a channel containing cylinders (confined cylinders). The CFD and experimental geometries and inlet and boundary conditions are identical and model the geometries found within a nuclear reactor core. Validation of the CFD models is assessed and it is found that while some models can accurately predict the time-varying quantities considered, the majority demonstrate deficiencies. Higher fidelity models typically predict these quantities with increased accuracy. The uncertainty for both the computational and experimental results are estimated and discussed. Uncertainty estimation of both CFD and experimental results is required for meaningful validation. However, uncertainty from the non-invasive velocity measurement technique, particle image velocimetry (PIV), is inadequate for validation purposes, particularly random time-varying flow fluctuations (turbulence). Within this dissertation, the uncertainty from four dominant error sources are demonstrated, calculated, and analyzed for PIV. This method of estimating instantaneous, mean, and fluctuation uncertainty for PIV is demonstrated with significant accuracy and is applied to the confined cylinders experimental results for the validation study.

This book introduces novel design techniques developed to increase the safety of aircraft engines. The authors demonstrate how the application of uncertainty methods can overcome problems in the accurate prediction of engine lift, caused by manufacturing error. This in turn ameliorates the difficulty of achieving required safety margins imposed by limits in current design and manufacturing methods. This text shows that even state-of-the-art computational fluid dynamics (CFD) are not able to predict the same performance measured in experiments; CFD methods assume idealised geometries but ideal geometries do not exist, cannot be manufactured and their performance differs from real-world ones. By applying geometrical variations of a few microns, the agreement with experiments improves dramatically, but unfortunately the manufacturing errors in engines or in experiments are unknown. In order to overcome this limitation, uncertainty quantification considers the probability density functions of manufacturing errors. It is then possible to predict the overall variation of the jet engine performance using stochastic techniques. Uncertainty Quantification in Computational Fluid Dynamics and Aircraft Engines demonstrates that some geometries are not affected by manufacturing errors, meaning that it is possible to design safer engines. Instead of trying to improve the manufacturing accuracy, uncertainty quantification when applied to CFD is able to indicate an improved design direction. This book will be of interest to gas turbine manufacturers and designers as well as CFD practitioners, specialists and researchers. Graduate and final year undergraduate students may also find it of use.

This book introduces design techniques developed to increase the safety of aircraft engines, and demonstrates how the application of stochastic methods can overcome problems in the accurate prediction of engine lift caused by manufacturing error. This in turn addresses the issue of achieving required safety margins when hampered by limits in current design and manufacturing methods. The authors show that avoiding the potential catastrophe generated by the failure of an aircraft engine relies on the prediction of the correct behaviour of microscopic imperfections. This book shows how to quantify the possibility of such failure, and that it is possible to design components that are inherently less risky and more reliable. This new, updated and significantly expanded edition gives an introduction to engine reliability and safety to contextualise this important issue, evaluates newly-proposed methods for uncertainty quantification as applied to jet engines. Uncertainty Quantification in Computational Fluid Dynamics and Aircraft

Engines will be of use to gas turbine manufacturers and designers as well as CFD practitioners, specialists and researchers. Graduate and final year undergraduate students in aerospace or mathematical engineering may also find it of interest.

With Applications to Computational Fluid Dynamics

Computational Fluid and Solid Mechanics 2003

Proceedings of the 32nd IMAC, A Conference and Exposition on Structural Dynamics, 2014

Presented at the Fluids Engineering Conference, Washington, D.C., June 20-24, 1993

Computational Fluid Dynamics Applied to Waste-to-Energy Processes

**This monograph presents computational techniques and numerical analysis to study conservation laws under uncertainty using the stochastic Galerkin formulation. With the continual growth of computer power, these methods are becoming increasingly popular as an alternative to more classical sampling-based techniques. The text takes advantage of stochastic Galerkin projections applied to the original conservation laws to produce a large system of modified partial differential equations, the solutions to which directly provide a full statistical characterization of the effect of uncertainties. Polynomial Chaos Methods of Hyperbolic Partial Differential Equations focuses on the analysis of stochastic Galerkin systems obtained for linear and non-linear convection-diffusion equations and for a systems of conservation laws; a detailed well-posedness and accuracy analysis is presented to enable the design of robust and stable numerical methods. The exposition is restricted to one spatial dimension and one uncertain parameter as its extension is conceptually straightforward. The numerical methods designed guarantee that the solutions to the uncertainty quantification systems will converge as the mesh size goes to zero. Examples from computational fluid dynamics are presented together with numerical methods suitable for the problem at hand: stable high-order finite-difference methods based on summation-by-parts operators for smooth problems, and robust shock-capturing methods for highly nonlinear problems. Academics and graduate students interested in computational fluid dynamics and uncertainty quantification will find this book of interest. Readers are expected to be familiar with the fundamentals of numerical analysis. Some background in stochastic methods is useful but not necessary.**

**"The Point Collocation Non-Intrusive Polynomial Chaos (NIPC) method was applied to a stochastic synthetic jet actuator problem to demonstrate the integration of computationally efficient uncertainty quantification to the high-fidelity CFD modeling of Synthetic Jet Actuators. The uncertainty quantification approach was first implemented in two stochastic model problem cases for the prediction of peak exit plane velocity using a Fluid Dynamic Based analytical model of the Synthetic Jet Actuator, which is computationally less expensive than CFD simulations. The NIPC results were compared with direct Monte Carlo sampling results. To demonstrate the efficient uncertainty quantification in CFD modeling of synthetic jet actuators, a test case, Case 1 (synthetic jet issuing into quiescent air), was selected from the CFDVal2004 workshop. In the stochastic CFD problem, the NIPC method was used to quantify the uncertainty in the long-time averaged  $u$  and  $v$ -velocities at several locations in the flow field, due to the uncertainty in the amplitude and frequency of the oscillation of the piezo-electric membrane. Fifth order NIPC expansions were used to obtain the uncertainty information which showed that the variation in the  $v$ -velocity is high in the region directly above the jet slot and the variation in the  $u$ -velocity is maximum in the region immediately adjacent to the slot. Even with a ten percent variation in the amplitude and frequency, the long-time averaged  $u$  and  $v$ -velocity profiles could not match the experimental measurements at  $y = 0.1\text{mm}$  above the slot, indicating that the discrepancy may be due to other uncertainty sources in CFD or measurement errors. A global sensitivity analysis using linear regression approach indicated that the frequency had a stronger contribution to the overall uncertainty in the long-time averaged flow field velocity for the range of input uncertainties considered in this study. Overall, the results obtained in this study showed the potential of Non-Intrusive Polynomial Chaos as an effective uncertainty quantification method for computationally expensive high-fidelity CFD simulations applied to the stochastic modeling of synthetic jet flow fields"--Abstract, leaf iii.**

**Computational fluid dynamics (CFD) simulations are becoming an increasingly important tool across a wide range of engineering disciplines. CFD simulations improve the accuracy and predictive capability of the evaluation process through numerical solution of the Reynolds-Averaged form of the Navier-Stokes (RANS) equations describing fluid flow.**

**Uncertainty arises in CFD simulations due to a variety of sources, and this uncertainty must be rigorously quantified in order to be useful in support of reactor licensing and decision making. In traditional system thermal hydraulics codes, the code scaling, applicability, and uncertainty (CSAU) approach is used to ensure simulation quality and to estimate the level of uncertainty present. No such method is presently available for CFD. This thesis discusses the pathway for utilizing CFD in reactor licensing applications in the face of uncertainty through the introduction of CFD-CSAU. In order to do this, modifications to the CSAU method are proposed to bring the process in line with requirements of CFD. This includes processes to ensure the quality of a simulation which are utilized in the CFD verification and validation community, but which are not currently utilized. In addition to ensuring simulation quality and confidence, a rigorous estimate of simulation uncertainty must be made. Emphasis is placed on the quantification of turbulence modeling uncertainty in a predictive context, as it is the clear missing link in the handling of CFD uncertainty. Previous work has commonly focused on the propagation of uncertainty due to turbulence model calibration coefficients, however such an approach ignores much of the uncertainty associated with the turbulence model, and does not extrapolate well to a full variety of flow conditions. In this work, a novel approach is discussed which is based on treating the uncertainty directly through the turbulent viscosity field ( $\mu_t$ ). This allows for a more complete treatment of the modeling uncertainty compared to the uncertainty in the calibration coefficients. As the turbulent viscosity takes on unique values in continuous space, the uncertainty must be modeled as a random field, defined by the marginal distribution and the covariance function. These properties are defined through two unique hyper-parameters, which are**

inferred on a training data set and applied to a variety of validation data sets. The approach is shown to generalize well to a wide variety of turbulent test cases in the accurate prediction of uncertainty bounds especially as compared to previous methods. The applicability for a representative reactor flow condition is demonstrated.

**Computational Fluid Dynamics Applied to Waste-to-Energy Processes: A Hands-On Approach** provides the key knowledge needed to perform CFD simulations using powerful commercial software tools. The book focuses on fluid mechanics, heat transfer and chemical reactions. To do so, the fundamentals of CFD are presented, with the entire workflow broken into manageable pieces that detail geometry preparation, meshing, problem setting, model implementation and post-processing actions. Pathways for process optimization using CFD integrated with Design of Experiments are also explored. The book's combined approach of theory, application and hands-on practice allows engineering graduate students, advanced undergraduates and industry practitioners to develop their own simulations. Provides the skills needed to perform real-life simulation calculations through a combination of mathematical background and real-world examples, including step-by-step tutorials Presents worked examples in complex processes as combustion or gasification involving fluid dynamics, heat and mass transfer, and complex chemistry sets

**Uncertainty Quantification Integrated to Computational Fluid Dynamic Modeling of Synthetic Jet Actuators**

**Efficient Uncertainty Quantification in Computational Fluid Dynamics**

**Quantification of Uncertainty in Aerodynamic Heating of a Reentry Vehicle Due to Uncertain Wall and Freestream Conditions**

**Polynomial Chaos Methods for Hyperbolic Partial Differential Equations**

**Foundational Aspects and Numerical Methods**

In recent decades, kinetic theory - originally developed as a field of mathematical physics - has emerged as one of the most prominent fields of modern mathematics. In recent years, there has been an explosion of applications of kinetic theory to other areas of research, such as biology and social sciences. This book collects lecture notes and recent advances in the field of kinetic theory of lecturers and speakers of the School "Trails in Kinetic Theory: Foundational Aspects and Numerical Methods", hosted at Hausdorff Institute for Mathematics (HIM) of Bonn, Germany, 2019, during the Junior Trimester Program "Kinetic Theory". Focusing on fundamental questions in both theoretical and numerical aspects, it also presents a broad view of related problems in socioeconomic sciences, pedestrian dynamics and traffic flow management.

This book explores recent advances in uncertainty quantification for hyperbolic, kinetic, and related problems. The contributions address a range of different aspects, including: polynomial chaos expansions, perturbation methods, multi-level Monte Carlo methods, importance sampling, and moment methods. The interest in these topics is rapidly growing, as their applications have now expanded to many areas in engineering, physics, biology and the social sciences. Accordingly, the book provides the scientific community with a topical overview of the latest research efforts.

Currently, computational fluid dynamics (CFD) is widely used in the nuclear thermal hydraulics field for design and safety analyses. To validate CFD codes, high quality multi dimensional flow field data are essential. The Matched Index of Refraction (MIR) Flow Facility at Idaho National Laboratory has a unique capability to contribute to the development of validated CFD codes through the use of Particle Image Velocimetry (PIV). The significance of the MIR facility is that it permits non intrusive velocity measurement techniques, such as PIV, through complex models without requiring probes and other instrumentation that disturb the flow. At the heart of any PIV calculation is the cross-correlation, which is used to estimate the displacement of particles in some small part of the image over the time span between two images. This image displacement is indicated by the location of the largest peak. In the MIR facility, uncertainty quantification is a challenging task due to the use of optical measurement techniques. Currently, this study is developing a reliable method to analyze uncertainty and sensitivity of the measured data and develop a computer code to automatically analyze the uncertainty/sensitivity of the measured data. The main objective of this study is to develop a well established uncertainty quantification method for the MIR Flow Facility, which consists of many complicated uncertainty factors. In this study, the uncertainty sources are resolved in depth by categorizing them into uncertainties from the MIR flow loop and PIV system (including particle motion, image distortion, and data processing). Then, each uncertainty source is mathematically modeled or adequately defined. Finally, this study will provide a method and procedure to quantify the experimental uncertainty in the MIR Flow Facility with sample test results.

"The primary focus of this study is to demonstrate an efficient approach for uncertainty quantification of surface heat flux to the spherical non-ablating heatshield of a generic reentry vehicle due to epistemic and aleatory uncertainties that may exist in various parameters used in the numerical solution of hypersonic, viscous, laminar blunt-body flows with thermo-chemical non-equilibrium. Two main uncertainty sources were treated in the computational fluid dynamics (CFD) simulations: (1) aleatory uncertainty in the freestream velocity and (2) epistemic uncertainty in the recombination efficiency for a partially catalytic wall boundary condition. The Second-Order Probability utilizing a stochastic response surface obtained with Point-Collocation Non-Intrusive Polynomial Chaos was used for the propagation of mixed (aleatory and epistemic) uncertainties. The uncertainty quantification approach was validated on a stochastic model problem with mixed uncertainties for the prediction of stagnation point heat transfer with Fay-Riddell relation, which included the comparison with direct Monte Carlo sampling results. In the stochastic CFD problem, the uncertainty in surface heat transfer was obtained in terms of intervals at different probability levels at various locations including the stagnation point and the shoulder region. The mixed uncertainty results were compared to the results obtained with a purely aleatory uncertainty analysis to show the difference between two uncertainty quantification approaches. A global sensitivity analysis indicated that the velocity has a stronger contribution to the overall uncertainty in

the stagnation point heat transfer for the range of input uncertainties considered in this study"--Abstract, leaf iii.

Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification

Inherent and Model-form Uncertainty Analysis for CFD Simulation of Synthetic Jet Actuators

Trails in Kinetic Theory

Assessing the Reliability of Complex Models

Development of Carbonaceous Chemistry for Computational Modeling (C3M) with Application of Uncertainty Quantification (UQ) Analysis for Coal

Gasification Kinetics in Computational Fluid Dynamics (CFD) Modeling

*During the last decade, research in Uncertainty Quantification (UC) has received a tremendous boost, in fluid engineering and coupled structural-fluids systems. New algorithms and adaptive variants have also emerged. This timely compendium overviews in detail the current state of the art of the field, including advances in structural engineering, along with the recent focus on fluids and coupled systems. Such a strong compilation of these vibrant research areas will certainly be an inspirational reference material for the scientific community. Computational fluid dynamics (CFD) has been widely studied and used in the scientific community and in the industry. Various models were proposed to solve problems in different areas. However, all models deviate from reality. Uncertainty quantification (UQ) process evaluates the overall uncertainties associated with the prediction of quantities of interest. In particular it studies the propagation of input uncertainties to the outputs of the models so that confidence intervals can be provided for the simulation results. In the present work, a non-intrusive quadrature-based uncertainty quantification (QBUQ) approach is proposed. The probability distribution function (PDF) of the system response can be then reconstructed using extended quadrature method of moments (EQMOM) and extended conditional quadrature method of moments (ECQMOM). The report first explains the theory of QBUQ approach, including methods to generate samples for problems with single or multiple uncertain input parameters, low order statistics, and required number of samples. Then methods for univariate PDF reconstruction (EQMOM) and multivariate PDF reconstruction (ECQMOM) are explained. The implementation of QBUQ approach into the open-source CFD code MFIX is discussed next. At last, QBUQ approach is demonstrated in several applications. The method is first applied to two examples: a developing flow in a channel with uncertain viscosity, and an oblique shock problem with uncertain upstream Mach number. The error in the prediction of the moment response is studied as a function of the number of samples, and the accuracy of the moments required to reconstruct the PDF of the system response is discussed. The QBUQ approach is then demonstrated by considering a bubbling fluidized bed as example application. The mean particle size is assumed to be the uncertain input parameter. The system is simulated with a standard two-fluid model with kinetic theory closures for the particulate phase implemented into MFIX. The effect of uncertainty on the disperse-phase volume fraction, on the phase velocities and on the pressure drop inside the fluidized bed are examined, and the reconstructed PDFs are provided for the three quantities studied. Then the approach is applied to a bubbling fluidized bed with two uncertain parameters, particle-particle and particle-wall restitution coefficients. Contour plots of the mean and standard deviation of solid volume fraction, solid phase velocities and gas pressure are provided. The PDFs of the response are reconstructed using EQMOM with appropriate kernel density functions. The simulation results are compared to experimental data provided by the 2013 NETL small-scale challenge problem. Lastly, the proposed procedure is demonstrated by considering a riser of a circulating fluidized bed as an example application. The mean particle size is considered to be the uncertain input parameter. Contour plots of the mean and standard deviation of solid volume fraction, solid phase velocities, and granular temperature are provided. Mean values and confidence intervals of the quantities of interest are compared to the experiment results. The univariate and bivariate PDF reconstructions of the system response are performed using EQMOM and ECQMOM.*

*This book presents the state-of-the-art in supercomputer simulation. It includes the latest findings from leading researchers using systems from the High Performance Computing Center Stuttgart (HLRS) in 2019. The reports cover all fields of computational science and engineering ranging from CFD to computational physics and from chemistry to computer science with a special emphasis on industrially relevant applications. Presenting findings of one of Europe's leading systems, this volume covers a wide variety of applications that deliver a high level of sustained performance. The book covers the main methods in high-performance computing. Its outstanding results in achieving the best performance for production codes are of particular interest for both scientists and engineers. The book comes with a wealth of color illustrations and tables of results.*

*Uncertainty Quantification in Computational Fluid Dynamics* Springer Science & Business Media

*Unsteady Computational Fluid Dynamics (CFD) Validation and Uncertainty Quantification for a Confined Bank of Cylinders Using Particle Image Velocimetry (PIV)*

*Gradient-based Approaches for Sensitivity Analysis and Uncertainty Quantification Within Hypersonic Flows*

*Uncertainty Quantification in Computational Fluid Dynamics*

***Efficient and Robust Uncertainty Quantification for Computational Fluid Dynamics and Fluid-structure Interaction  
Transactions of the High Performance Computing Center, Stuttgart (HLRS) 2019***

Fluid flows are characterized by uncertain inputs such as random initial data, material and flux coefficients, and boundary conditions. The current volume addresses the issue of efficiently computing the flow uncertainty, given this initial randomness. It collects seven original review articles that cover improved versions of the Monte Carlo (the so-called multi-level Monte Carlo method (MLMC)), moment-based stochastic Galerkin methods and modified versions of the stochastic collocation methods that use adaptive stencil selection of the ENO-WENO type in both physical and stochastic space. The methods are also complemented by concrete applications such as flows around aerofoils and rockets, problems of aeroelasticity (fluid-structure interactions), and shallow water flows for propagating water waves. The wealth of numerical examples provides evidence on the suitability of each proposed method as well as comparisons of different approaches.

This book covers cutting-edge findings related to uncertainty quantification and optimization under uncertainties (i.e. robust and reliable optimization), with a special emphasis on aeronautics and turbomachinery, although not limited to these fields. It describes new methods for uncertainty quantification, such as non-intrusive polynomial chaos, moment-based methods, perturbation methods, as well as adjoint based and multi-level Monte Carlo methods. It includes methods for characterization of most influential uncertainties and formulations for robust and reliable design optimization. A distinctive element of the book is the unique collection of test cases with prescribed uncertainties, which are representative of the current engineering practice of the industrial consortium partners involved in UMRIDA, a level 1 collaborative project within the European Commission's Seventh Framework Programme (FP7). All developed methods are benchmarked against these industrial challenges. Moreover, the book includes a section dedicated to Practice Guidelines for uncertainty quantification and robust design optimization, summarizing the findings obtained by the consortium members within the UMRIDA project. In all, the book offers a authoritative guide to cutting-edge methodologies for uncertainty management in engineering design, covers a wide range of applications and discusses ideas for future research and interdisciplinary collaborations.

This report presents the state of advancement of a Nuclear Energy Advanced Modeling and Simulation (NEAMS) project to characterize the uncertainty of the computational fluid dynamics (CFD) code Nek5000 using the Dakota package for flows encountered in the nuclear engineering industry. Nek5000 is a high order spectral element CFD code developed at Argonne National Laboratory for high resolution spectral-filtered large eddy simulations (LESs) and unsteady Reynolds averaged Navier-Stokes (URANS) simulations.

With the proliferation of simulation within the design and analysis of engineering systems, uncertainty quantification and sensitivity analysis have taken on increased importance, providing valuable information for assessing the reliability of simulation outputs and a means for improving these results. In this work, uncertainty quantification and sensitivity analysis within the context of hypersonic computational fluid dynamics is examined. The simulation of hypersonic flows relies on numerous constitutive relations to account for chemical reactions, internal energy modes and molecular transport. Within these constitutive relations are hundreds of constants and parameters, which are often the result of experimental measurements. The goal of sensitivity analysis is determining the simulation parameters most affecting an output of interest, while the goal of uncertainty quantification is determining the variability of simulation outputs resulting from the uncertainty associated with model parameters. Traditional methods for uncertainty quantification and sensitivity analysis typically rely on exhaustive sampling, where hundreds to thousands of simulations are performed and relevant statistics are computed. For complex simulations, these exhaustive approaches are prohibitively expensive and well beyond the computational budget of most projects. For this work, gradient-based methods are used to reduce the expense of uncertainty quantification and sensitivity analysis. Using an adjoint-based approach, the derivative of an output with respect to simulation parameters can be computed in a constant amount of work, providing more information about the simulation output without a significant increase in cost. This additional information can then be leveraged in novel ways, such as surrogate models or optimization, to accelerate the process of uncertainty quantification or sensitivity analysis. This dissertation demonstrates these gradient-based methods for sensitivity analysis and uncertainty quantification in hypersonic flow simulations and assesses the performance of these methods in terms of cost and accuracy.

Uncertainty Quantification for Hyperbolic and Kinetic Equations

Dakota Uncertainty Quantification Methods Applied to the NEK-5000 SAHEX Model

Model Validation and Uncertainty Quantification, Volume 3

Advancements in Uncertainty Quantification with Stochastic Expansions Applied to Supersonic and Hypersonic Flows

Uncertainty Quantification in Computational Fluid Dynamics and Aircraft Engines

Advances in computing hardware and algorithms have dramatically improved the ability to simulate complex processes computationally. Today's simulation capabilities offer the prospect of addressing questions that in the past could be addressed only by resource-intensive experimentation, if at all. Assessing the Reliability of Complex Models recognizes the ubiquity of uncertainty in computational estimates of reality and the necessity for its quantification. As computational science and engineering have matured, the process of quantifying or bounding uncertainties in a computational estimate of a physical quality of interest has evolved into a small set of interdependent tasks: verification, validation, and uncertainty of quantification (VVUQ). In recognition of the increasing importance of computational simulation and the increasing need

to assess uncertainties in computational results, the National Research Council was asked to study the mathematical foundations of VVUQ and to recommend steps that will ultimately lead to improved processes. Assessing the Reliability of Complex Models discusses changes in education of professionals and dissemination of information that should enhance the ability of future VVUQ practitioners to improve and properly apply VVUQ methodologies to difficult problems, enhance the ability of VVUQ customers to understand VVUQ results and use them to make informed decisions, and enhance the ability of all VVUQ stakeholders to communicate with each other. This report is an essential resource for all decision and policy makers in the field, students, stakeholders, UQ experts, and VVUQ educators and practitioners.

The life of engine components is determined by a combination of the material properties and the applied stresses and temperatures. As a consequence of variability in these parameters, the component life is not fixed (deterministic) but stochastic (random) and may be characterised by a probability density function (PDF). In order to reduce the cost of ownership of ADF aircraft these PDFs need to be determined as accurately as possible. Probabilistic techniques offer significant potential for accurate and realistic estimates of component lives by quantifying stochastic elements of an analysis rather than introducing excessive conservatism to allow for them. This report examines the feasibility of using a probabilistic approach for modelling the component temperatures in an engine using CFD (Computational Fluid Dynamics).

This third volume of eight from the IMAC - XXXII Conference, brings together contributions to this important area of research and engineering. The collection presents early findings and case studies on fundamental and applied aspects of Structural Dynamics, including papers on: Linear Systems Substructure Modelling Adaptive Structures Experimental Techniques Analytical Methods Damage Detection Damping of Materials & Members Modal Parameter Identification Modal Testing Methods System Identification Active Control Modal Parameter Estimation Processing Modal Data

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Uncertainty Quantification in Multiscale Materials Modeling

Dakota Uncertainty Quantification Methods Applied to the CFD Code Nek5000

Probabilistic Prognostics and Health Management of Energy Systems

Quantification of Uncertainty in Computational Fluid Dynamics

This report summarizes the results of a NEAMS project focused on the use of uncertainty and sensitivity analysis methods within the NEK-5000 and Dakota software framework for assessing failure probabilities as part of probabilistic risk assessment. NEK-5000 is a software tool under development at Argonne National Laboratory to perform computational fluid dynamics calculations for applications such as thermohydraulics of nuclear reactor cores. Dakota is a software tool developed at Sandia National Laboratories containing optimization, sensitivity analysis, and uncertainty quantification algorithms. The goal of this work is to demonstrate the use of uncertainty quantification methods in Dakota with NEK-5000.

Findings and Best Practice Collected During UMRIDA, a Collaborative Research Project (2013–2016) Funded by the European Union

Uncertainty Quantification Tools for Multiphase Gas-Solid Flow Simulations Using Mfix

Computational Fluid Dynamics and Turbulence Model Uncertainty Quantification for Nuclear Reactor Safety Applications

A Hands-On Approach

Special Issue