Journal of the Mechanics and Physics of Solids 72 (2014) 1–19

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Optimal uncertainty quantification with model uncertainty and legacy data

P.-H.T. Kamga, B. Li, M. McKerns, L.H. Nguyen, M. Ortiz, H. Owhadi, T.J. Sullivan *

Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125, USA

ARTICLE INFO

Article history:
Received 19 July 2013
Received in revised form
1 July 2014
Accepted 17 July 2014
Available online 2 August 2014

Keywords:
Hypervelocity impact
Uncertainty quantification
Optimal transportation
Meshfree interpolation
Particle erosion

ABSTRACT

We present an optimal uncertainty quantification (OUQ) protocol for systems that are characterized by an existing physics-based model and for which only legacy data is available, i.e., no additional experimental testing of the system is possible. Specifically, the OUQ strategy developed in this work consists of using the legacy data to establish, in a probabilistic sense, the level of error of the model, or *modeling error*, and to subsequently use the *validated model* as a basis for the determination of probabilities of outcomes. The quantification of *modeling uncertainty* specifically establishes, to a specified confidence, the probability that the actual response of the system lies within a certain distance of the model. Once the extent of model uncertainty has been established in this manner, the model can be conveniently used to stand in for the actual or empirical response of the system in order to compute probabilities of outcomes. To this end, we resort to the *OUQ reduction theorem* of Owhadi et al. (2013) in order to reduce the computation of optimal upper and lower bounds on probabilities of outcomes to a *finite-dimensional optimization* problem. We illustrate the resulting UQ protocol by means of an application concerned with the response to hypervelocity impact of 6061-T6 Aluminum plates by Nylon 6/6 impactors at impact velocities in the range of 5–7 km/s. The ability of the legacy OUQ protocol to process diverse information on the system and its ability to supply rigorous bounds on system performance under realistic—and less than ideal—scenarios demonstrated by the hypervelocity impact application is remarkable.

1. Introduction

The principal objective of the present work is the formulation of a rigorous uncertainty quantification (UQ) protocol for systems characterized by a fixed data set, or *legacy data*, and by a physics-based model of unknown and uncertain fidelity, as well as with the formulation of efficient methods of solution and approximation thereof. By uncertainty quantification we specifically mean the determination of *probabilities of outcomes* in systems whose response is stochastic or uncertain, be it as a result of intrinsic randomness in the system, randomness in its inputs or operating conditions, epistemic uncertainty about system operation, or a combination thereof. A case in point concerns *system certification*, i.e., the assessment of the probability that a system will perform safely and within specifications. The system is certified if the probability of failure to

* Corresponding author.
E-mail addresses: ortiz@aero.caltech.edu (M. Ortiz), Tim.Sullivan@warwick.ac.uk (T.J. Sullivan).

http://dx.doi.org/10.1016/j.jmps.2014.07.007

perform safely is below a prespecified failure tolerance ϵ. In addition, we wish to establish the *confidence* that we may place on a given certification assessment, i.e., we wish to ascertain the frequency with which the certification may be expected to be correct. Thus, we say that a system is certified with probability of failure ϵ, or probability of success $1-\epsilon$, and confidence $1-\epsilon'$ if the assessment that a system will perform successfully with probability $1-\epsilon$ is correct with probability $1-\epsilon'$. Specifically, a way to test the preceding statement empirically is: (i) perform the certification assessment a large number of times; (ii) for every certification assessment, test the system a large number of times and establish whether the certification assessment is correct, i.e., whether the system indeed fails with probability less than ϵ; (iii) verify that the fraction of certifications that are correct is at least $1-\epsilon'$. In practice, we often desire *both* ϵ and ϵ' to be small numbers, i.e., we wish to certify with great confidence that the failure rate of the system is small. Indeed, a system can always be certified on the basis of overly optimistic assumptions regarding its performance, but the confidence in such a certification should be correspondingly low. Conversely, insisting on a very high level of confidence in the certification assessment is bound to render certification unlikely. It is precisely the antagonistic demands of low failure tolerance and high certification confidence that make rigorous certification challenging and, in particular, place stringent requirements on experiment, modeling and uncertainty quantification.

In practice, a number of difficulties prevent the direct evaluation of the probability of failure of a system. For instance, the input space is often of very high dimension and some of the input parameters are unknown (the so-called *unknown unknowns*). In addition, the probability measure of the known inputs—let alone the exact values of realizations of those inputs—is often not fully known. Many systems exhibit responses that are (or appear to be) stochastic in nature, and are controlled by physical processes whose functional form is only imperfectly characterized either by experiment or theory. Physical and computational models of the system may exist, but often these models are only partially verified and validated. In some cases, some of the underlying physics may be inadvertently omitted from the models or may not be covered by existing theory. This imperfect knowledge of the functional form of the response of the system is sometimes referred to as *model uncertainty*, and it constitutes a major source of uncertainty in practice. The situation is often compounded for systems whose performance cannot be fully tested, either because the operating conditions cannot be reproduced in the laboratory, or because the tests are costly, or subject to environmental or treaty restrictions, or some combination thereof. Often, legacy or archival data exists but is incomplete, inconsistent and noisy. Moreover, the mechanisms responsible for the failure of systems are often rare events and thus not directly accessible to simple Monte Carlo sampling; this inaccessibility makes it difficult to characterize their physical and probabilistic properties from experimental evidence. Finally, the failure of some systems is of great consequence, be it economic or in loss of life, and the tolerance for failure is correspondingly low. Here again, the tension between imperfect and incomplete information about the system and the desire to prevent rare but exceedingly costly failures during operation makes rigorous uncertainty quantification challenging in practice.

This work specifically considers systems that are characterized by an existing physics-based model and for which only legacy data is available, i.e., no additional experimental testing of the system is possible. The use of models for the design, assessment and certification of engineering systems is, evidently, standard. In addition, modeling and simulation is often less costly than experimental testing and lends itself to more extensive and systematic parametric studies. It is therefore desirable that a UQ protocol make maximum use of existing models while simultaneously ensuring rigorous and testable probabilities of outcomes and confidence levels in the assessment. Situations in which only legacy data is available also arise commonly in practice, e.g., in surveillance programs instituted to monitor the health of deployed systems, specially when a significantly abnormal condition is encountered in the field, and in the redesign of systems. In these cases, the questions of whether the existing data provide sufficient coverage of the system under abnormal conditions, or of the redesigned system, and the extent to which designs can be 'extrapolated' away from the legacy data base, are of central concern.

The UQ strategy adopted in this work consists of using the legacy data to establish, in a probabilistic sense, the level of error of the model, or *modeling error*, and to subsequently use the *validated model* as a basis for the determination of probabilities of outcomes. The quantification of *modeling uncertainty* specifically establishes, to a specified confidence, the probability that the actual response of the system, which may depend on hidden or unaccounted-for variables, lies within a certain distance of the model. Once the extent of model uncertainty has been established in this manner, the model can be conveniently used to stand in for the actual or empirical response of the system in order to compute probabilities of outcomes. Evidently, in this approach model uncertainty compounds uncertainties due to the intrinsic randomness of the system or to the randomness of the inputs. Therefore, in practice the success and the proposed UQ protocol depends critically on the fidelity of the model and the quality and extent of the data. Once the model has been validated, and the model uncertainty has been quantified, we compute bounds on probabilities of outcomes by recourse to optimal uncertainty quantification (OUQ) (Owhadi et al., 2013). In particular, we resort to the *reduction theorem* of Owhadi et al. (2013) in order to reduce the computation of optimal upper and lower bounds on probabilities of outcomes to a *finite-dimensional optimization* problem.

We illustrate the resulting UQ protocol by means of an application concerned with the response to hypervelocity impact of 6061-T6 Aluminum plates by Nylon 6/6 impactors at impact velocities in the range of 5–7 km/s. Hypervelocity impact sets in motion complex physics that challenge modeling and simulation, both as regards material modeling and solvers. The system under consideration is characterized by three input parameters, namely, impact velocity, plate thickness, and obliquity, and the outcome of interest (i.e., quantity of interest) is the perforation area. The resulting UQ problem concerns, therefore, the determination of bounds on perforation area probabilities when the system is allowed to operate over a certain range of the input parameters. Experimental data in support of the UQ analysis is obtained at Caltech's Small Particle