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Predictive modeling methodology for obtaining optimally predicted results with reduced uncertainties: Illustrative application to a simulated solar collector facility

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Abstract

This work illustrates the application to a simulated solar collector facility of a recently developed, comprehensive, predictive modeling methodology for obtaining optimally predicted best-estimate results, with reduced uncertainties. The application of the very efficient adjoint sensitivity analysis methodology (*ASAM*) for nonlinear systems is also illustrated by computing exactly the first-order sensitivities of selected facility responses to all model parameters. These sensitivities are used to rank the importance of parameters in contributing to response uncertainties, and also serve within the predictive methodology as the weighting functions for propagating uncertainties of the model parameters and for assimilating measurements and simulations. The results produced by the predictive modeling procedure are optimally predicted values for the responses and for all model parameters, with reduced predicted uncertainties that are smaller than either the measured or the computed uncertainties. The amount of reduction is controlled by the magnitude of the respective sensitivities: the larger the magnitude of the sensitivities, the larger the reduction in the predicted uncertainties.

The predictive methodology presented in this work can be used for validating simulation models, and for designing and/or improving the performance of experimental installations. Current limitations of this predictive modeling methodology are also highlighted, along with ongoing work towards generalizing and significantly extending its applicability.

Keywords: Solar collector; Adjoint sensitivity analysis; Predictive modeling; Data assimilation; Model calibration; Best-estimate predictions with reduced uncertainties

1. Introduction

The solar thermal collector (STC) is an essential component of a solar thermal system, acting as a heat exchanger to convert solar irradiance into internal energy of the transport material flowing through the collector. Experimental and theoretical evaluations of various collector performances have been richly addressed in the literature, e.g., Benz and Beikircher (1999), Fischer et al. (2004), Kalogirou (2004, 2006), Duffy and Beckman (2006), Kratzenberg et al. (2006), Rojas et al. (2008), Sözen et al. (2008), Zambolin and Del Col (2010), Ayompe et al. (2011), Ayompe and Duffy (2013a, 2013b), and Xu et al. (2012).

Although many works have evaluated the performance of STCs, relatively few have investigated the effects of uncertainties (see, e.g., Kratzenberg et al., 2006), or have

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used experimental information explicitly for improving the modeling of STCs (see, e.g., Kalogirou, 2006). As is well known, the results of measurements inevitably reflect the influence of experimental errors. On the other hand, computations are afflicted by errors stemming from numerical procedures, uncertain model parameters, boundary and initial conditions, and/or imperfectly known physical processes. Therefore, nominal values for experimentally measured and/or computed quantities are insufficient, by themselves, for applications. The quantitative uncertainties accompanying the measurements and computations are also needed, along with the respective nominal values. Extracting "best estimate" values for model parameters and predicted results (responses), together with "best estimate" uncertainties for these parameters and responses requires the combination of experimental and computational data and accompanying uncertainties. Such a combination process requires reasoning from incomplete, error-afflicted, and occasionally discrepant information.

Differences between experimental and computational results provide the basic motivation for performing quantitative model verification, validation, and predictive modeling. Loosely speaking, "*code/model verification*" seeks quantitative answers to the question "is the mathematical model solved correctly?" "*Code/model validation*" seeks quantitative answers to the question "does the model represent reality?", comparing computational with experimental results (including computed and experimental uncertainties in these results). The initial stage of *predictive modeling* is to quantify the uncertainties from all steps in the sequence of modeling and simulation processes that lead to a computational model prediction. Typical uncertainties stem from: (a) data biases and uncertainties in all model parameters (including initial and/or boundary conditions, external forcing functions, correlations, etc.), (b) numerical errors, and (c) uncertainties due to lack of perfect knowledge of the processes being modeled. The second step is to compute the sensitivities (i.e., the 1st-order functional derivatives) of the responses of interest to all the uncertain model parameters. The next step is to integrate all available experimental and/or additional computational data for the purpose of updating the parameters of the model ("model calibration") under investigation, and for producing optimally predicted results, with reduced predicted uncertainties. Important issues to be addressed include the estimation of discrepancies in the data, and of the biases between model predictions and experimental data. The state-of-the-art of data assimilation and model calibration methods require a very significant computational effort. Reducing this computational effort is greatly facilitated by using the *adjoint sensitivity analysis method* (*ASAM*) for nonlinear systems, which was introduced by Cacuci (1981a, 1981b, 2003; see also Faragó et al., 2013). The results of the predictive modeling analysis are probabilistic descriptions of possible future outcomes based on all available information, including errors and uncertainties.

Cacuci and Ionescu-Bujor (2010) have recently published a comprehensive *predictive modeling* methodology for predicting optimal best-estimate values for model responses and parameters (following the assimilation experimental data and simultaneous calibration of model parameters and responses), along with reduced predicted uncertainties, for large-scale nonlinear time-dependent systems. This predictive modeling methodology includes, as particular cases, the "4D-VAR" data assimilation procedures used in the geophysical sciences (see, e.g., Faragó et al., 2013; Cacuci et al., 2005, 2013), and also provides a quantitative indicator, constructed from sensitivity and covariance matrices, for determining the consistency (agreement or disagreement) among the a priori computational and experimental data.

This work presents an application of the predictive modeling methodology developed by Cacuci and Ionescu-Bujor (2010) to a simulated paradigm facility for analyzing the efficiency of solar collectors. The computational modeling of the simulated paradigm facility is presented in Section 2. Section 3 presents the sensitivity analysis of typical computed and/or measured responses to the model parameters characterizing the simulator. Notably, the response sensitivities are computed using the very efficient "*adjoint sensitivity analysis methodology* (*ASAM*)" originally developed by Cacuci (1981a, 1981b). These sensitivities are used to rank the importance of parameters in contributing to response uncertainties. In Section 4 of this work, these sensitivities are also shown to play a fundamental role as "weighting functions" for assimilating additional experimental and/or computational data to obtain "best-estimate" predicted values for the responses and the model parameters. It will also be shown that the predicted uncertainties in the predicted responses and model parameters are reduced to values that are smaller than either the experimentally measured or the computed uncertainties. The amount of reduction in the predicted uncertainties is controlled by the magnitude of the respective sensitivities: the larger the magnitude of the sensitivities, the larger the reduction in the predicted uncertainties. Finally, Section 5 highlights the usefulness of the predictive modeling methodology for validating simulation models, and for designing and/or improving the performance of experimental installations. Current limitations of the predictive modeling methodology (Cacuci and Ionescu-Bujor, 2010) used in this work also discussed along with ongoing work aimed at alleviating these limitations, which would significantly extending this methodology's applicability.

2. Mathematical modeling of a paradigm facility for measuring collector efficiency

Flat-plate collectors (FPC) are widely used due to their lower relative costs and easy handling (Rabl 1985). This Section presents the modeling of a paradigm digital facility