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Comparison of global sensitivity analysis methods – Application to fuel behavior modeling

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HIGHLIGHTS

- Several global sensitivity analysis methods are compared.
- The methods' applicability to nuclear fuel performance simulations is assessed.
- The implications of large input uncertainties and complex models are discussed.
- Alternative strategies to perform sensitivity analyses are proposed.

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ABSTRACT

Fuel performance codes have two characteristics that make their sensitivity analysis challenging: large uncertainties in input parameters and complex, non-linear and non-additive structure of the models. The complex structure of the code leads to interactions between inputs that show as cross terms in the sensitivity analysis. Due to the large uncertainties of the inputs these interactions are significant, sometimes even dominating the sensitivity analysis. For the same reason, standard linearization techniques do not usually perform well in the analysis of fuel performance codes. More sophisticated methods are typically needed in the analysis. To this end, we compare the performance of several sensitivity analysis methods in the analysis of a steady state FRAPCON simulation. The comparison of importance rankings obtained with the various methods shows that even the simplest methods can be sufficient for the analysis of fuel maximum temperature. However, the analysis of the gap conductance requires more powerful methods that take into account the interactions of the inputs. In some cases, moment-independent methods are needed. We also investigate the computational cost of the various methods and present recommendations as to which methods to use in the analysis.

1. Introduction

Light water reactor fuel performance codes model the behavior of the fuel rod under irradiation, either in the steady state or in transient conditions. The purpose of the modeling is to provide understanding about how the thermal, mechanical and materials properties interact and how the rod responds as a whole to the boundary conditions imposed by the environment. An important aspect of the analyses is to support the rod design and safe operation, so that the rod cladding remains intact and various safety margins are respected. In addition to the usual difficulty of representing a complex system with soluble mathematical models, there are also large uncertainties in many of the system and model parameters. Therefore sensitivity analyses are often coupled with uncertainty analyses, which take into account the uncertainties in the code input, and produce an estimate of the uncertainty of the calculated result. To take the analysis one step further, one may ask how to reduce the uncertainty of the results, or which of the code inputs is responsible for the uncertainty of the result. These questions can be addressed by sensitivity analysis.

The goal of a sensitivity analysis is to find the most influential input parameter to the computed model output. The method chosen for the sensitivity analysis depends on the computational cost of the model, the number of inputs to be considered, and the specific question to be answered by the analysis. Although adjoint-based methods have been implemented into fuel performance codes in the past (Christensen et al., 1981; Wilderman and Was, 1984), the more generic, sampling-based methods are typically used nowadays. Of these, computationally the most inexpensive method is the one-at-a-time (OAT) method, where each parameter is

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varied independently while keeping the others fixed (Geelhood et al., 2009; Sagrado and Herranz, 2013). Although often used due to its simplicity, the method suffers from poor coverage of the parameter space and from lack of control over the quality of the analysis (Saltelli et al., 2010). For a typical fuel performance code, such as FRAPCON (Geelhood et al., 2011a,b), the computational time per run is of the order of seconds or minutes. Therefore using Monte Carlo based sensitivity analysis methods is entirely feasible. They have been adopted in many studies to perform global sensitivity analyses (Glaeser, 2008; Boulore et al., 2012; Ikonen and Tulkki, 2014; Pastore et al., 2015). Global sensitivity analysis methods have the advantage of exploring the whole parameter space (hence the term global), and in general can be used to identify properties of very complex models. It should be mentioned that in addition to Monte Carlo based evaluation, global sensitivity analysis can also be performed with computationally more lenient methods (Sudret, 2008).

In this work, we study the practical aspects of using some of the most common global Monte Carlo based sensitivity analysis methods. We apply variance based methods, including the Pearson correlation analysis (Draper and Smith, 1998), and the Sobol' variance decomposition (Sobol', 1993). These methods are based on estimating the influence of a given input on the output variance. A closely related method is the elementary effects method (Morris, 1991), which is the global extension of the OAT method. In certain cases it is possible that the variance or other moments of the probability distribution is not a good measure of uncertainty. Then, moment-independent methods can be used. In this work, we employ the density-based Borgonovo δ measure (Borgonovo, 2007), for which an efficient estimation method was recently introduced by Plischke et al. (2013).

Another consideration when choosing the method is the specific question posed to the analysis. Questions such as "If we could eliminate the uncertainty of one input parameter, which one should we choose in order to reduce the variance of the output as much as possible?" and "Which of the input parameters are so non-influential that they can be fixed?" define the setting of the sensitivity analysis (Saltelli and Saisana, 2007; Saltelli et al., 2008). The first one corresponds to factor prioritization (FP) and the second one to factor fixing (FF) setting. In the FP setting, a good starting point is to determine the main (first order) effect of an input parameter. Higher-order analysis is needed in models with dominating interaction terms (uncertainties in the output that only arise as a result of changing more than one variable simultaneously). Also in the FF setting one has to consider the interactions between different inputs. These can be quantified, for example, by the total effect sensitivity index T_i, the elementary effects method, or in part by the Borgonovo δ measure, discussed in Section 2.

For a fuel performance code, the role of interactions in the model can be significant (Ikonen and Tulkki, 2014). This is because of two characteristics of fuel performance codes: large uncertainties in input parameters and complex, non-linear and non-additive structure of the models. A famous example of the latter is the gap conductance, which couples together the thermal, mechanical and microstructural (e.g., fission gas release) models in the fuel performance code. The intertwined structure of the code leads to interactions between inputs that show as cross terms in the sensitivity analysis. Due to the large uncertainties of the inputs these interactions are significant, sometimes even dominating the sensitivity analysis. For the same reason, standard linearization techniques do not usually perform well in the analysis of fuel performance codes.

A thorough sensitivity analysis of a fuel performance code requires methods that can cope with the large uncertainties and interactions. On the other hand, the simplicity and computational ease of the OAT method is very appealing. In this work, we attempt to address the choice between different methods by comparing their performance in the sensitivity analysis of a steady state scenario modeled with the FRAPCON-3.4 code. In our analysis we focus on the maximum fuel temperature and the gap conductance computed for a mid-burnup (22 MWd/kgU) PWR rod. The latter is particularly challenging to analyze and showcases the potential caveats of the simple methods. We also briefly study the convergence and required computational effort of the methods.

2. Analysis methods

2.1. One-at-a-time (OAT) analysis

Arguably the simplest sensitivity analysis strategy is to vary one model input parameter at a time while keeping the others fixed. Typically such a one-at-a-time (OAT) sampling is done around the nominal (most probable, or best estimate) values of the input parameters. It is possible to choose the sampling points in many ways, but one of the most common ones is to choose the extreme values of the distribution (Sagrado and Herranz, 2013). Another typical way would be to evaluate the effect of infinitesimal changes to the inputs by choosing a very small deviation from the nominal value. However, in the case of a fuel performance code, where we do not expect the model to linearize effectively and where the uncertainties are large, we choose to sample the parameters at their extreme values. One could of course increase the number of points to sample intermediate values of the parameter (Pastore et al., 2015). While this increases the likelihood of catching non-monotonic effects of the input parameters, it also quickly increases the number of required function evaluations, and is unlikely to cover the parameter space efficiently (Saltelli and Annoni, 2010).

The change in the model output is evaluated at all the sampled points, and the input causing the largest change in the output is given the highest rank in the sensitivity analysis. In this work, we define the OAT sensitivity measure for input X_i as

$$OAT_i = \frac{\max_{\mathbf{\Delta}_i} |f(\mathbf{X}+\mathbf{\Delta}_i) - f(\mathbf{X})|}{\sum_i (\max_{\mathbf{\Delta}_i} |f(\mathbf{X}+\mathbf{\Delta}_i) - f(\mathbf{X})|)}, \quad (1)$$

where $\mathbf{X}$ is the vector of the nominal values of the inputs, and $\mathbf{\Delta}_i$ is a vector of zeros, except for its ith element $\Delta_i^{(i)}$, which is chosen so that $X_i + \Delta_i^{(i)}$ gives the extrema of the distribution of X_i. The maximum is taken over these two extrema. The function f represents one of the outputs of the computer code. The denominator serves to normalize the measure so that it can be easily compared to the global sensitivity measures discussed below, which are normalized between 0 and 1 by construction. The normalization has no effect on the parameter ranking.

The computational cost of the method is very small, as the number of required simulation runs is only $2k+1$, where k is the number of inputs.

2.2. Global sensitivity analysis

The goal of global sensitivity analysis is to characterize the dependence of the model output on its inputs in the whole input parameter space. Usually the analysis involves some kind of Monte Carlo sampling of the inputs, either by pseudo random sampling or by quasi random sampling. In quasi random sampling, the sample points are chosen in a way that avoids clusters and results in more effective sampling and faster convergence. In this work, the Sobol' quasi random sequence (Sobol', 1967) is used to generate the sample points. The variables U_i generated by the Sobol' sequence uniformly partition the unit interval (0, 1). The inverse cumulative distribution function (ICDF) method is used to map them to the actual input variables X_i according to $X_i = P_i^{-1}(U_i)$, where P_i