Sensitivity Analysis and Bayesian Calibration of OpenSees Models using quoFEM

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Abstract. The NHERI SimCenter is a nine-year research project that aims to advance the simulation of natural hazard impact on the built environment and communities. The SimCenter is developing several open-source workflow applications and an underlying scientific application framework. All applications built on this framework provide an OpenSees interface that enables users to use their existing models in advanced simulation studies, such as local and regional performance assessment, and uncertainty quantification (UQ). SimCenter applications provide researchers an opportunity to explore different extensions of their models by lowering the interdisciplinary barrier and encouraging collaboration. Among the applications, quoFEM provides access to UQ analyses with an easy-to-use, standardized interface. This work demonstrates the research enabled by quoFEM through the example of model calibration using PM4Sand, a soil constitutive model available in OpenSees. After an initial sensitivity analysis, the model is calibrated using Bayesian inference based on observations of hysteretic soil response from cyclic direct simple shear tests. The uncertainty in the model parameters is used in forward propagation to explore plausible lateral spreading scenarios due to seismic liquefaction. The results demonstrate the utility of quoFEM to the OpenSees community as a UQ-enabling tool.

Keywords: SimCenter, quoFEM, DesignSafe, uncertainty quantification, Bayesian calibration, PM4Sand, liquefaction, global sensitivity analysis

1 Introduction

Although uncertainties in computer simulation models can have substantial influence on the accuracy and bias of model predictions [1], the uncertainty in model parameters and outputs are rarely quantified and characterized in natural hazards engineering research and practice. This is only partly explained by the computational resource demands: uncertainty quantification (UQ) typically requires hundreds or thousands of model evaluations. Another important challenge is implementing efficient algorithms that support state-of-the-art techniques for sensitivity analyses, calibration, and propagation of uncertainties and combining these algorithms with applications used in natural hazards engineering, e.g. finite element applications. These implementations often involve sophisticated tuning schemes that are tailored to the context and type of model being used, with researchers sometimes needing to develop robust interfaces between tasks. For example, investigating the liquefaction of a site subjected to earthquake excitation involves at least two steps: (1) uncertainty reduction by optimizing parameters using a measurement model; (2) uncertainty propagation by simulating site response using a system prediction model. Such series of tasks is commonly applied in natural hazards engineering (NHE) [2].

The NHERI SimCenter is an NSF-funded nine-year research project aiming to build a collaborative simulation platform for researchers in the NHE community. This platform connects various models, data, and UQ algorithms to facilitate the design and execution of complex workflows which solve various user-specific problems using computational simulation [3]. The SimCenter develops a collection of open-source desktop applications built on top of one shared underlying application framework. Each desktop application is specialized to support a particular context and the corresponding problem types and scales in NHE, e.g. from the response of an individual building to response of all the buildings in a region. The SimCenter's cloud-enabled application framework encompasses every step in the broad natural hazard impact assessment workflow, from source/asset description to regional loss/recovery simulation. Each step of the workflow is covered by one or more available workflow applications. Since, the workflow applications responsible for structural response estimation support user-defined OpenSees [4] models, such models can be imported and used in every SimCenter desktop application with minimal effort.

quoFEM (Quantified Uncertainty with Optimization for the Finite Element Method) is a SimCenter desktop application that focuses on providing practical and robust UQ algorithms that can be readily applied to user-defined simulation models [5]. The application provides an interface with OpenSees and other simulation applications. It connects users with the high-performance computing resources at the Texas Advanced Computing Center through the DesignSafe cyberinfrastructure to support the resource-intensive UQ calculations. The graphical user interface facilitates setting up a UQ analysis and testing different plausible characterizations for the random variables to better understand the model behavior under uncertainty.

This paper first provides a brief overview of quoFEM followed by a case study to demonstrate the utility of the application through a probabilistic soil model calibration problem. Parameters of the PM4Sand liquefaction-capable constitutive model [6,7] in OpenSees are calibrated using Cyclic Direct Simple Shear (CyDSS) lab test data [8,9]. Given the model and the dataset, quoFEM was used to perform a series of probabilistic analyses: (1) global sensitivity analysis to identify the primary/trivial model parameters that influence the onset of liquefaction [10]; (2) Bayesian calibration of model parameters using the transitional Markov chain Monte Carlo (TMCMC) algorithm [11]; and (3) forward analysis to propagate the remaining uncertainties in the material model through an OpenSees simulation of the lateral spreading of a soil-column under an earthquake scenario.

2 quoFEM

2.1 SimCenter workflows

The workflows supported by SimCenter tools are a series of interconnected workflow applications that can be illustrated with the jigsaw puzzle pieces in Fig. 1 that are based on the main components of the performance-based engineering (PBE) paradigm [12]. Each SimCenter desktop application uses different subsets of the available workflow applications to create workflows. The R2D Tool (Region Resilience Determination), for example, spans the full range from asset and hazard description to recovery simulation, while WE-UQ (Wind Engineering with UQ) covers only the (wind) event simulations, structural modeling and response estimation, and corresponding uncertainty quantification (UQ) parts. Response estimation and UQ are the common core that is used across all desktop applications. quoFEM is the fundamental SimCenter application that is built on this common core as shown in the right side of Fig. 1.

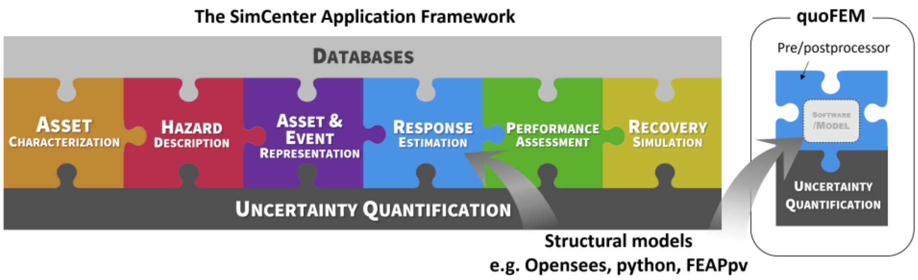

Fig. 1. The SimCenter application framework and quoFEM

2.2 Supported UQ algorithms

quoFEM is designed to facilitate UQ analyses on a wide range of deterministic/black-box simulation models. The currently implemented UQ methods are selected considering their utility in the natural hazards engineering context and the demand and feedback received from NHE researchers. quoFEM (v3.1.0) currently supports global sensitivity analysis, reliability analysis, Bayesian parameter calibration, surrogate modeling, along with Monte Carlo-type forward propagation and deterministic optimization techniques. Each type of UQ analysis is supported by different methods. The developers of novel UQ algorithms can use the custom-UQ option to incorporate their techniques into quoFEM. This makes the tool a collaborative research platform that connects UQ experts and engineering model developers.

2.3 Interfacing with Finite Element Codes

Currently, four model engine interfaces are supported: (1) OpenSees using Tcl files to describe the model [4]; (2) Generic Python scripts that support OpenSeesPy as well as Python wrappers around any other executable [13], (3) FEAPpv [14], and (4) Surrogate models. A fifth, custom driver option allows researchers to write their own interface. Using the built-in OpenSees interfaces involves only the following two steps:

(1) **Define input random variables**: The random variables of the model are identified by using a `pset` command instead of the typical `set` command in the model script. The probability distributions corresponding to the random variables can be specified through the graphical user interface.

(2) **Process outputs and prepare quantities of interest**: A post-processing script needs to be prepared that reads the recorder outputs of OpenSees and calculates the response quantities of interest. These values need to be written as an array in a `results.out` text file.

2.4 High Performance Computing through DesignSafe

All SimCenter applications provide convenient access to high performance computing resources through the DesignSafe cyberinfrastructure, hosted at the Texas Advanced Computing Center (TACC, 2020). quoFEM analyses can run either locally at the user's computer or remotely at DesignSafe. The same user interface of the desktop application is used to set up both types of analyses and users can switch to run a remote calculation by simply selecting the remote running option. After specifying the desired number of processors to use, the input files are automatically prepared and sent to one of the HPCs at TACC and the job is immediately submitted to the queue. The built-in parallelized UQ algorithms efficiently utilize multiple processing cores and the scaling potential provided by the HPC cluster.

There are also other, advanced options available to launch remote jobs.
Fig. 2 provides a summary of these options: (1) The desktop application is accessible through a web browser using graphical remote application streaming and the NICE DCV client in DesignSafe. This service provides the user experience of a desktop application without installing anything on the local machine. (2) The Jupyter Hub environment on DesignSafe allows researchers to control runs through Python scripts that specify job variables and submit the job through the Tapis system at DesignSafe. In such a Jupyter notebook, the remote UQ analysis through quoFEM can be treated as one function in a larger routine, e.g., reliability-based optimizations. This approach is provided for advanced users who seek to extend the tool or use pre-defined scripts to run a large number of analyses.

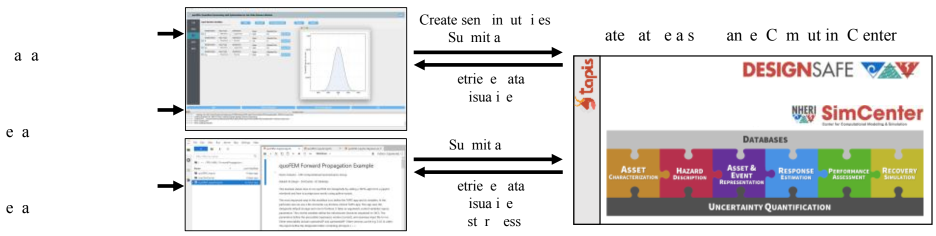

Fig. 2. Running quoFEM analysis using remote computing resources at DesignSafe

3 Sensitivity Analysis and Bayesian Calibration of a Constitutive Soil Model using quoFEM

3.1 Problem description

This illustrative example demonstrates several UQ techniques using the parameters of the PM4Sand constitutive model [6,7], a liquefaction-capable soil model in OpenSees. This complex material model is often calibrated using a small number of experimental results which yields imperfect information about its parameters, and this leads to uncertain model predictions. Quantifying such uncertainties and inspecting the uncertainty bounds of model predictions can provide more information about the importance of each model parameter. Recognizing these uncertainties can incentivize more sophisticated modeling and calibration techniques that can better utilize the available data from experiments to reduce these bounds and provide more robust and higher fidelity simulations.

In this study, the amount of reduction in the uncertainty in PM4Sand parameters calibrated to Cyclic Direct Simple Shear (CyDSS) test data is inspected, and the resulting uncertainty is propagated in an earthquake excitation simulation of a soil column. Three steps of UQ analyses are presented:

- **Global sensitivity analysis** to get an insight into which parameters are critical in triggering liquefaction. This is an important first step to check if a given dataset is useful for calibrating the parameters of interest.
- **Bayesian calibration** to obtain the posterior probability distribution of the PM4Sand parameters based on the CyDSS test dataset.
- **Forward propagation** to investigate how the uncertainty that remains after the Bayesian calibration (characterized by the posterior probability distribution) affects the prediction of an earthquake response.

The PM4Sand constitutive model has 24 parameters. Among the parameters, apparent relative density D_r, shear modulus coefficient G_o, and contraction rate parameter h_{po}, are known to be important for predicting liquefaction responses [6]. Therefore, these three parameters $\boldsymbol{\theta}=\{D_r,G_o,h_{po}\}$ are considered in the UQ analyses and their prior distributions are assumed to be uniform distributions with the ranges shown in Table 1. These prior distributions shall capture a plausible wide range that includes all possible

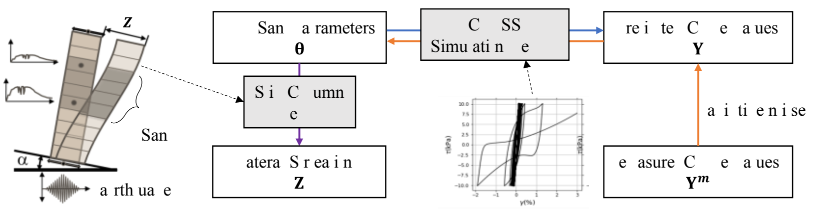

Fig. 3. Probabilistic calibration of soil model (step 2) with sensitivity analysis (step 1) and prediction of uncertainty in seismic liquefaction (step 3)

parameter values for the target soils. The experimental data will be used to constrain this wide range to the domain that best describes the behavior exhibited by the specimen during the experiments. The following three analyses were set up using the quoFEM graphical user interface and run on the HPC at DesignSafe utilizing 200 processors.

Table 1. Prior distributions of PM4Sand parameters

Parameter	Distribution	Range
D_r	Uniform	0.1-0.6
G_o	Uniform	200-2000
h_{po}	Uniform	0.01-5

3.2 Step 1 – Global Sensitivity Analysis

The sensitivity analysis is performed for a simulation model that reproduces the CyDSS test. The output quantity of interest is the number of cycles until the onset of liquefaction (denoted as Y). The onset of liquefaction is defined as the time step when the shear strain exceeds 3.5%. Liquefaction capacity is also affected by vertical compression typically characterized by the cyclic shear stress ratio (CSR; i.e., ratio of horizontal cyclic shear stress to vertical consolidation stress). In this sensitivity analysis, a CSR of 0.175 is considered. Two variance-based global sensitivity indices are evaluated:

$$S_i = \frac{\mathbb{V}\mathrm{ar}_{\theta_i}\left[\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}\left[Y \mid \theta_i\right]\right]}{\mathbb{V}\mathrm{ar}_{\boldsymbol{\theta}}\left[Y\right]} \tag{1}$$

$$S_i^T = \frac{\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}\left[\mathbb{V}\mathrm{ar}_{\theta_i}\left[Y \mid \boldsymbol{\theta}_{\sim i}\right]\right]}{\mathbb{V}\mathrm{ar}_{\boldsymbol{\theta}}\left[Y\right]} \tag{2}$$

where θ_i is the parameter of interest (i.e., one of the $\{D_r,G_o,h_{po}\}$), $\boldsymbol{\theta}_{\sim i}$ denotes the other two parameters, $\mathbb{E}_{\mathbf{X}}[\bullet]$ and $\mathbb{V}\mathrm{ar}_{\mathbf{X}}[\bullet]$ denotes mean and variance of function over $\mathbf{X}$, respectively, and the vertical bar denotes 'conditional n' . The former index, called the main-effect index, quantifies how much of the variance of Y is attributed to the parameter θ_i, while the latter index, called the total-effect index, also considers the joint contributions of θ_i and other parameters [10].

The sensitivity analysis is performed using the algorithm in Weirs et al. (2012) through the Dakota engine that interfaces with quoFEM [10]. 2500 simulations were performed using the prior distributions in Table 1 . The resulting sensitivity is shown in Fig. 4(a) which indicates that D_r is the dominating parameter for the response Y. This is also confirmed by inspecting the scatter plot of Fig. 4(b): D_r (horizontal axis) demonstrates a stronger influence on the output (vertical axis) compared to the influence of the other parameters shown in (c) and (d). Based on this, we can expect that the CyDSS observations will help constrain the uncertainty in D_r, while the reduction of uncertainty in h_{po} and G_o will be relatively limited. Additional, different types of experiments would be needed to better characterize those other parameters.

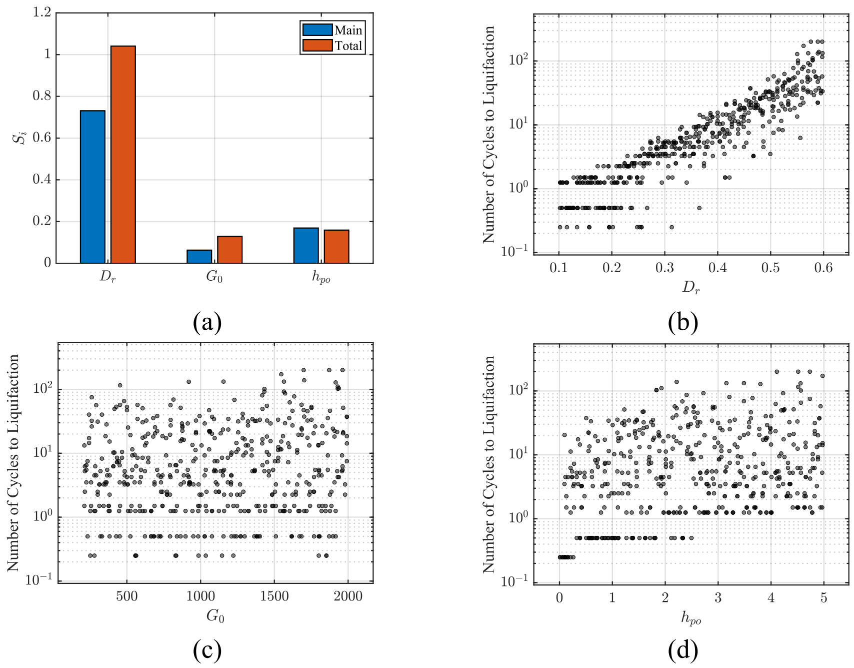

Fig. 4. (a) Sensitivity analysis results for the critical number of cycles given CSR= 0.172; (b)-(d) Individual input-output scatter plots

3.3 Step 2 – Bayesian Parameter Calibration

Consider now the observations of the CyDSS experiment in Table 2, that are publicly available on the DesignSafe data depot [8,9]. We assume that the observed count of cycles at different CSR values, denoted as Y_i^m (i=1,…,6), is given by the simulation model predictions and an added Gaussian noise. The latter captures various inaccuracies such as inherent uncertainty in the phenomenon, the imperfection of our simulation model, and measurement error. Given the above assumptions, we can denote the relationship between the data and model prediction, $Y_i(\boldsymbol{\theta})$, as

$$Y_i^m = Y_i(\boldsymbol{\theta}) + \varepsilon_i \tag{3}$$

where noise ε_i is assumed to have zero-mean and unknown variance $\sigma_{\varepsilon,i}^2$. Given the six measurement values, we can use a Bayesian approach to evaluate the posterior distribution of the parameters of PM4Sand and the unknown noise variances:

$$p(\boldsymbol{\theta}, \boldsymbol{\sigma}_\varepsilon^2 \mid Y_1^m, .., Y_6^m) = \frac{1}{c} \prod_{i=1}^{6} p(Y_i^m \mid \boldsymbol{\theta}, \sigma_{\varepsilon,i}^2) p(\boldsymbol{\theta}) p(\boldsymbol{\sigma}_\varepsilon^2) \tag{4}$$

where $p\cdot$ denotes the (joint) probability distribution, and c is the normalization constant that ensures the area under the posterior distribution is one. From Eq. (3),

Table 2. Cyclic direct simple shear (CyDSS) test experimental data

Cyclic shear stress ratio (CSR)	Number of cycles to onset of liquefaction
0.105	26
0.105	21
0.130	13
0.151	5
0.172	4
0.200	3

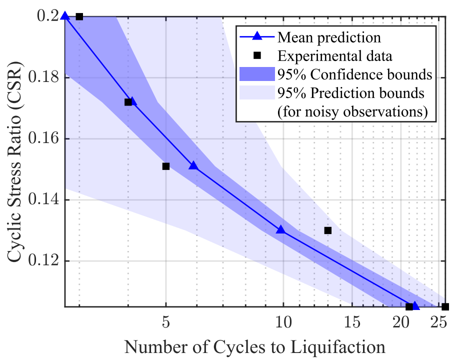

Fig. 5. Comparison of calibrated model predictions and experimental data

$p(Y_i^m \mid \boldsymbol{\theta}, \sigma_i^2)$ is a Gaussian distribution with mean $Y_i(\boldsymbol{\theta})$ and variance of σ_i^2. The prior distribution of $\boldsymbol{\theta}$ is in Table 1. Following best practices, inverse Gamma priors with the shape parameter α=3 and scale parameter β=2 are introduced for the σ_i^2 measurement variances [15]. The posterior sample of $\boldsymbol{\theta}$ in this example is obtained using the transitional Markov chain Monte Carlo (TMCMC) sampling technique [11] that is available in quoFEM through the UCSD-UQ engine. This is an expensive calculation that greatly benefits from the available HPC resources at DesignSafe.

Fig. 5 compares the experimental data with the calibrated model predictions of the load-cycle counts, while Fig. 6 shows the calibrated parameter sample from the joint posterior distribution. Fig. 6 shows that uncertainty in all variables is reduced by calibrating to the observed data, but the reduction was most apparent in D_r. This is in line with our expectations from the earlier sensitivity analysis. The results also highlight a strong dependency between D_r and h_{po}, indicating that multiple combinations of D_r and h_{po} produce near-optimal solutions. None of these features are captured by a deterministic estimator that results from a conventional error-minimizing optimization approach (e.g., red diamond marker shown in the same figure). It is also important to recognize that a non-negligible amount of uncertainty remains in the parameter estimates, and this produces substantial uncertainty in the model predictions. The dark blue bounds in Fig. 5 show the level of uncertainty in the estimated number of cycles to liquefaction, but this simulation model was prepared to reproduce the experimental setup. When the calibrated constitutive model is applied in another simulation, the responses can exhibit different scales of uncertainties. A forward propagation analysis is helpful to characterize such uncertainties in a simulation model. It is good practice to run such an analysis and characterize the effect of uncertainties on application-specific quantities of interest before practically applying these parameter values in a simulation for decision making.

3.4 Step 3 – Forward Propagation

The obtained samples of the soil parameters in Fig. 6 are used to predict the uncertainty in the lateral spreading response of a site subjected to an earthquake (Loma Prieta Gilroy Array #2) with peak ground acceleration of 0.37 g. The soil column model shown

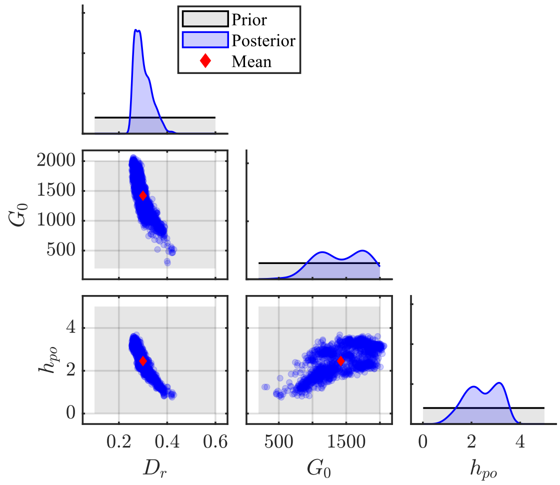

Fig. 6. PM4Sand model parameters sampled from the joint posterior distribution

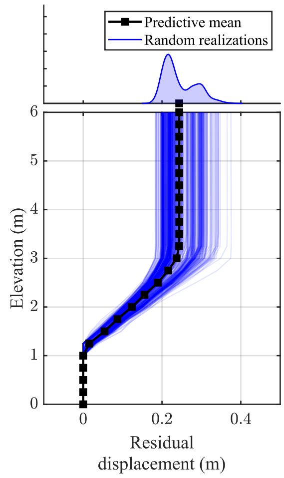

Fig. 7. Predicted earthquake response of soil column

in Fig. 3 is introduced in which the liquefiable layer in the middle is modeled using PM4Sand and the other parts are assumed to remain elastic throughout the shaking. The results of 500 simulations are shown in Fig. 7. The mean and standard deviation of the residual displacement at the surface level (6 m) are 0.24 m and 0.02 m, respectively. Depending on the application, the uncertainty in these results can be considered reasonably low. The sample of the predictive distribution shown on the top of the vertical profile can further be utilized in reliability and risk assessment workflows.

4 Concluding Remarks

The case study presented in this paper has shown how quoFEM could support a series of different UQ analyses to inspect the uncertain characteristics of a constitutive soil model in OpenSees. Sensitivity analysis suggested that the uncertainty in each parameters has a different contribution to the outputs. Consequently, we could predict that Bayesian calibration will provide disproportionate information and reducing the uncertainty in some of the parameters would require additional, different type of experiments. The uncertainty that remains after Bayesian calibration can be propagated through the response simulation to understand how it affects the outputs. The example has shown that the relationship between input and output uncertainties is not trivial.

Probabilistic analysis always provides a better understanding of the model behavior and associated physics than a deterministic approach. The SimCenter aims to accelerate the adoption of UQ techniques in the natural hazards engineering community by making robust and practical UQ algorithms more accessible to researchers and practitioners. All results shown in this work were obtained solely by quoFEM to emphasize that researchers can conveniently include such analyses in the scope of their work. quoFEM also supports further extension of the research scope to other UQ analyses, such as surrogate modeling and reliability analysis using the same model scripts.

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