Uncertainty Quantification of Building Performance Simulation using Gaussian Process Emulator and Polynomial Chaos Expansion

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ABSTRACT

Uncertainty Quantification (UQ) based on Monte Carlo Sampling (MCS) methods has been widely used for decision making problems. UQ is useful to address stochastic nature by quantifying risks of predicted outputs. However, for successful implementation of UQ, it takes significant modeling efforts and computation time.

For handling the aforementioned issue, this study introduces two meta-models (Gaussian Process Emulator [GPE] and Polynomial Chaos Expansion [PCE]) which can be regarded as a surrogate model of a dynamic whole-building simulation model. In this study, the GPE and PCE are compared in terms of prediction capability and model flexibility under the different number of training data and inputs. In the paper, it is discussed whether two meta-models would be able to produce high performance qualities with acceptable computation time.

KEYWORDS

Uncertainty Quantification, Monte Carlo Sampling, Gaussian Process, Polynomial Chaos, Building simulation

INTRODUCTION

Uncertainty Quantification (UQ) has been widely used for stochastic performance assessments of various systems in building environments. UQ based on Monte Carlo Sampling (MCS) methods can easily identify the risks embedded in the simulation domain. This will help to unveil the problems hidden within the simulation domain, and produce meaningful and trustworthy probabilistic results compared to the deterministic approach. Nevertheless, some building experts still believe that the predicted outputs of the simulation tools can be used, without considering uncertainty sources as undeniably accurate decision making information for solving real problems. This is partly because the increased computational burdens of the simulation tools for the uncertainty propagation act as a significant obstacle to adopting the stochastic approach, considering the limited time and budget in reality. To reduce these

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computational burdens, meta-models (Gaussian Process Emulator (GPE) and Polynomial Chaos Expansion (PCE)) have been put forward. The abilities of GPE and PCE for reliable performance assessments under uncertainty have been substantiated. However, comparative study of GPE and PCE in the building simulation domain has yet to be carried out.

This paper addresses these two meta-models (GPE and PCE) for a simulation tool (EnergyPlus), which are then tested in terms of their probabilistic prediction abilities and model flexibility. The test was implemented by selecting different numbers of training data and inputs. For this study, an existing office building was chosen and the calibrated and the validated EnergyPlus model, examined in a previous study (Kim et al. 2014), is used as a dynamic simulation tool.

META MODELS

A GPE, which is a non-parametric black-box model, constructs a regression model using the input and output training dataset sampled from the simulation tool, Gaussian Process, and Bayesian inference. To obtain the sampled input/output training dataset, the simulation cases of the unknown inputs are constructed using sampling methods (Simple Random Sampling (SRS), Quasi-Random Sampling (QRS), Latin Hypercube Sampling (LHS), etc.) and the outputs are then calculated. The drawn training dataset can then be expressed as Gaussian Process with Gaussian noise by using the kernel function composed of the mean function and covariance function (Equations 1-4). The Gaussian process, which expresses a multivariate normal distribution with Gaussian noise, generally has a kernel function with zero mean function and covariance function.

$$k(x_i, x_j') = \begin{bmatrix} C(x_1, x_1) & \dots & C(x_1, x_n) \\ \dots & \dots & \dots \\ C(x_n, x_1) & \dots & C(x_n, x_n) \end{bmatrix} \tag{1}$$

$$f(x_i) \sim gp(m(x_i), k(x_i, x_j') \tag{2}$$

$$\varepsilon_i \sim N(0, v_t) \tag{3}$$

$$y_i = f(x_i) + \varepsilon_i \tag{4}$$

where $k(x_i, x_j')$ is kernel function, $C(x_i, x_j)$ is covariance function, gp is Gaussian process, $m(x_i)$ is mean function, ε_i is Gaussian noise, v_t is variance of the Gaussian noise.

A Squared Exponential (SE) covariance function based on stationary Gaussian Process was used. The SE covariance function includes hyperparameters such as the scaling parameter and length-scale parameter. And the variance of Gaussian noise, which is expressed to be a diagonal matrix, is a hyperparameter that is difficult to determine, similar to the aforementioned scaling parameter and length-scale parameter. The three aforementioned hyperparameters are important for the GPE, and the GPE requires appropriate parameter estimation. To obtain the posterior distribution of three hyperparameters, Maximum A Posteriori (MAP) estimation was chosen. The MAP estimation is suitable to obtain the posterior distribution using the prior distribution of hyperparameter and likelihood function.

A PCE, which is a set of basis functions obtained from hypergeometric orthogonal polynomials, has been used for uncertainty propagation in engineering problems (Hosder & Walters, 2010). The PCE can be classified as either an intrusive or non-intrusive method. The intrusive method requires algebraic manipulations in the mathematical equations for estimating polynomial coefficients for the polynomial basis functions using Galerkin projection. However, these modifications of a computer code can involve complicated tasks. On the other hand, the non-intrusive method deals with a black-box model, similar to the aforementioned GPE. Considering the uncertainty propagation of the high-fidelity models having complicated mathematical equations, the non-intrusive method involves less complicated tasks than the intrusive method. In this study, Point-collocation Non-Intrusive Polynomial Chaos (NIPC) was chosen. The point-collocation NIPC constructs a regression model using input and output training dataset as shown in Equation 5.

$$\begin{bmatrix} Y(\xi_1) \\ Y(\xi_2) \\ \vdots \\ Y(\xi_{N_c}) \end{bmatrix} = \begin{bmatrix} \Psi_0(\xi_1) & \Psi_1(\xi_1) & \cdots & \Psi_{N_c-1}(\xi_1) \\ \Psi_0(\xi_2) & \Psi_1(\xi_2) & \cdots & \Psi_{N_c-1}(\xi_2) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_0(\xi_{N_c}) & \Psi_1(\xi_{N_c}) & \cdots & \Psi_{N_c-1}(\xi_{N_c}) \end{bmatrix} \times \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{N_c-1} \end{bmatrix} \quad (5)$$

where $\Psi(\xi)$ is stochastic components of polynomial basis function, a_j is deterministic component of polynomial basis function.

TARGET BUILDING AND UNKNOWN INPUTS

A 5-story office building (floor area: 6,900 m^2) located in South Korea was chosen as shown in Figure 1. The EnergyPlus model was calibrated using Bayesian calibration, and was validated (Kim et al. 2014). The posterior distributions of the unknown inputs in the EnergyPlus model were obtained using the current design information of an existing building. But, if future design problems such as those in retrofits are given, the EnergyPlus model needs to simultaneously reflect random samples taken from the posterior distributions as well as future uncertain conditions. With the previous calibrated and validated EnergyPlus model, this study only focuses on the uncertainty propagation, considering future uncertain conditions. The 47 unknown inputs were chosen as shown in Table 1. The unknown inputs including future climate data and future retrofit inputs were selected by collaboration with various decision makers (designers, engineers, and simulationists). And the unknown inputs were assumed to have uniform distributions (U[0.9, 1.1]), which is the ratio against the calibrated inputs in the EnergyPlus model. The number of sampling was set to 200.

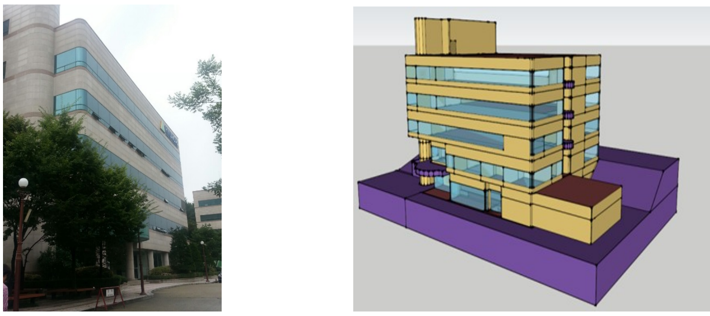


Figure 1. *Target building (left) and EnergyPlus displayed in OpenStudio (right)*

Table 1. *Comparison between EnergyPlus and GPM*

Classification		Details
Constructio n materials	x1-x3	Density, specific heat and conductivity of concrete.
	x4-x6	Density, specific heat and conductivity of mortar
	x7-x9	Density, specific heat and conductivity of concrete block
	x10-x12	Density, specific heat and conductivity of stone
	x13-x15	Density, specific heat and conductivity of insulation
	x16-x18	Density, specific heat and conductivity of insulation
	x19-x21	Density, specific heat and conductivity of board
	x22-x23	U-factor and SHGC of window 1
	x24-x25	U-factor and SHGC of window 2
	x26	Infiltration
Indoor loads	x27	Internal gain of lights
	x28	Internal gain of electric equipment
HVAC	x29-x31	Fan efficiency, pressure rise and motor efficiency of supply fans
	x32-x34	Fan efficiency, pressure rise and motor efficiency of return fans
Pump	x35-x36	Rated pump head and motor efficiency of chilled water pump
	x37-x38	Rated pump head and motor efficiency of condenser pump
	x39-x40	Rated pump head and motor efficiency of hot water pump
Plant	x41-x42	Heating and cooling COP of absorption chiller/heater #1
	x43-x44	Heating and cooling COP of absorption chiller/heater #2
Future climate data	x45	Prediction error of SRA1B scenario
	x46	Spatial downscaling error
	x47	Temporal downscaling error

The future climate data was generated using an ECHO-G model in Global Climate Models (GCM) proposed by IPCC (2007). The ECHO-G model provides the 20C3M scenario (climate during 100 years (1900-1999) since AD1900) for the 20th century run, and the SRA1B and SRA2 scenarios for future climate data (climate during 100 years (2000-2099) since AD2000 (IPCC, 2007). In this paper, the SRA1B scenario was chosen as the future climate data (2010-2030 years). However, the architectures of the ECHO-G model is inappropriate for the BPS tools due to spatial and temporal scaling problems. To solve the aforementioned issues, Inverse Distance Weighting (IDW) and Delta method were used as spatial and temporal downscaling methods, respectively. Moreover, horizontal global radiation was divided into direct and diffuse radiation using a direct and diffuse split model. However, it should be noted that the revised future climate data includes prediction errors of the SRA1B scenario for future climate change as well as numerical errors for spatial and temporal downscaling methods. In other words, the revised future climate data has three uncertain inputs. In addition, future retrofit inputs (construction materials, windows, infiltration, lights, electric equipment, supply/return fans, pumps, and plants) were chosen as uncertain inputs, since the inputs might have deteriorated or changed over the years.
The meta-models might provide low quality if the number of unknown inputs is greater than 10, due to the cures of dimensionality. Therefore, it is necessary to identify unknown inputs that have significant influence on the outputs. In this paper, the Standardized Rank Regression Coefficient (SRRC) method in the global sensitivity is used. Table 2 shows 5th ranking priority using the SRRC method. In the results, the future climate data and absorption chiller/heater were chosen as influential inputs. With the above sensitivity results, the meta-models were constructed into a regression model using the 5th ranking priority for inputs and gas energy consumption for outputs.

Table 2. *5th ranking priority using SRRC method*

No.	Priority	Sensitivity Index	Detail
x47	1	0.502	Temporal downscaling error
x46	2	0.499	Spatial downscaling error in the future climate data
x41	3	0.475	Heating COP of absorption chiller/heater #1
x45	4	0.473	Prediction error of SRA1B scenario
x42	5	0.359	Cooling COP of absorption chiller/heater #1

RESULTS

UQ is implemented using the meta-models (GPE and PCE) constructed based on the influential unknown inputs and gas energy consumption. To generate the selected input and output training dataset, the LHS method was used. The comparative study between the meta-models and the EnergyPlus was implemented where a different number of training datasets or different inputs and probability ranges are selected. Here, the number of samplings for obtaining the training dataset of the meta-models was set to 6, 12, 20, 30, and 42. Moreover, what-if scenarios with different inputs and probability ranges were selected as shown in Table 3. In other words, the aim of the comparative study is to test the prediction abilities of the meta-models with a different number of training datasets and a model flexibility when different inputs and probability ranges are selected.

To test the prediction abilities and model flexibility of the meta-models, the uncertainty results propagated by 200 simulation runs using the EnergyPlus model having 47 unknown inputs (Table 1) was used as the validation dataset. In addition, the empirical Cumulative Distribution Function (CDF) proposed by Helton & Davis (2003) and the two-sample Kolmogorov-Smirnov (K-S) hypothesis test were used for a comparison between the meta-models and EnergyPlus.

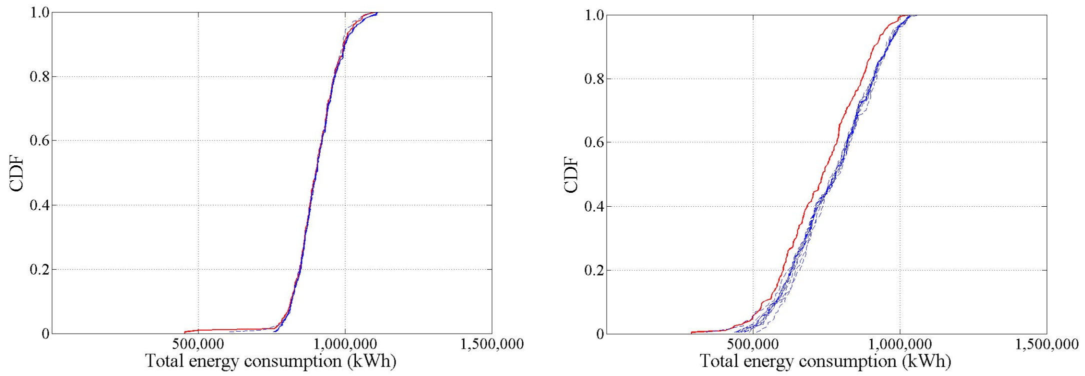
Table 3. *What-if scenarios*

Scenario	EnerygPlus Inputs		Uniform Probability Distribution	
	Heating COP	Cooling COP	Heating COP	Cooling COP
1	0.83	1.15	U[0.9, 1.1]	U[0.9, 1.1]
2	0.80	1.03	U[0.9, 1.1]	U[0.9, 1.1]
3	0.83	1.15	U[0.5, 1.2]	U[0.5, 1.2]
4	0.80	1.03	U[0.5, 1.2]	U[0.5, 1.2]

Figures 2-3 show the probabilistic predicted outputs based on the two empirical CDFs (EnergyPlus vs. meta-model) of two selected scenarios #1 and #4 having 5 (the number of unknown inputs) × 42 (the number of samplings) size. Tables 4-5 show the p-value results using the two-sample K-S hypothesis test. If the p-value is greater than 0.05, two CDFs is identical. Otherwise, the CDFs is not identical.

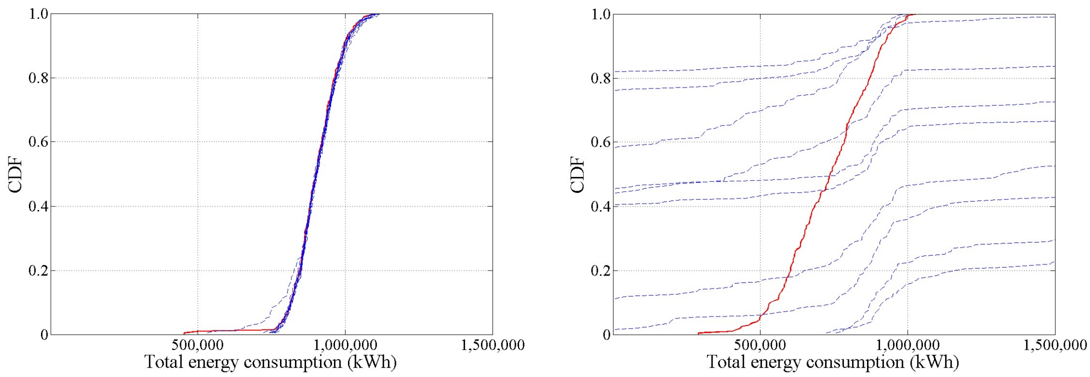
In the results of scenario #1 having the same inputs and probability ranges, the input and output training dataset increased, as the performance qualities of the two meta-models was improved as shown in Figures 2(a)-3(a). In addition, the minimum p-values based on the two-sample K-S hypothesis test were greater than 0.05 if the number of samplings are over 30 cases as shown in Tables 4-5. In other words, it can be inferred that the GPE and PCE can provide sufficiently meaningful probabilistic predicted outputs with fast computation time (around 1 or 2 seconds per simulation run) once more than around 30 input and output training dataset are sampled. Compared with the uncertainty propagation of the EnergyPlus model through 200 simulation runs (around 40 minutes per simulation run), this will be a considerable advantage.

As shown in Fig 2(b)-3(b), unlike the GPE, the PCE shows poor prediction abilities regardless of the number of samplings. In the case of scenarios #2-4 having different inputs and probability ranges, the minimum p-values of the PCE are less than 0.05. In contrast, the minimum p-values of GPE are greater than 0.05 if the number of samplings is greater than 30. In other words, the PCE can show very poor predicted outputs if the inputs or probability ranges significantly differ from the training dataset selected for constructing the PCE.



(a) Scenario #1 (b) Scenario #4

Figure 2. *GPE (blue) vs. EnergyPlus (red)*



(a) Scenario #1 (b) Scenario #4

Figure 3. *PCE (blue) vs. EnergyPlus (red)*

Table 4. *p-value results using two-sample K-S hypothesis test (EnergyPlus vs. GPE)*

Size	Scenario #1				Scenario #2				Scenario #3				Scenario #4			
	Mean	STD	Min	Max	Mean	STD	Min	Max	Mean	STD	Min	Max	Mean	STD	Min	Max
5×6	0.00	0.28	0.00	0.78	0.09	0.19	0.00	0.61	0.09	0.24	0.00	0.78	0.07	0.22	0.00	0.69
5×12	0.92	0.35	0.00	1.00	0.34	0.28	0.00	0.92	0.54	0.39	0.00	1.00	0.53	0.37	0.00	0.99
5×20	1.00	0.43	0.06	1.00	0.15	0.10	0.00	0.26	0.66	0.46	0.00	1.00	0.57	0.42	0.00	1.00
5×30	1.00	0.01	0.99	1.00	0.16	0.04	0.13	0.26	0.97	0.07	0.78	1.00	0.77	0.14	0.53	0.96
5×42	1.00	0.00	1.00	1.00	0.19	0.09	0.10	0.44	0.92	0.17	0.53	1.00	0.75	0.10	0.61	0.96

Table 5. *p-value results using two-sample K-S hypothesis test (EnergyPlus vs. PCE)*

Size	Scenario #1				Scenario #2				Scenario #3				Scenario #4			
	Mean	STD	Min	Max	Mean	STD	Min	Max	Mean	STD	Min	Max	Mean	STD	Min	Max
5×6	0.85	0.37	0.00	0.92	0.27	0.29	0.00	0.78	0.29	0.34	0.00	0.78	0.38	0.47	0.00	0.99
5×12	0.99	0.37	0.00	0.99	0.16	0.32	0.00	0.99	0.07	0.22	0.00	0.69	0.02	0.05	0.00	0.17
5×20	0.96	0.45	0.00	1.00	0.11	0.17	0.00	0.53	0.08	0.25	0.00	0.78	0.0	0.01	0.00	0.02
5×30	0.96	0.13	0.61	0.99	0.15	0.26	0.00	0.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5×42	1.00	0.15	0.53	1.00	0.08	0.22	0.00	0.69	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

CONCLUSIONS

This paper addressed two meta-models (GPE and PCE) for reducing the computation burden of BPS tools. And the probabilistic predicted outputs of the developed meta-models were compared with those of the EnergyPlus model.

In the results, the two meta-models provided excellent probabilistic predicted outputs compared to the developed basis model when the new inputs having identical inputs and probability ranges were used. In other words, the meta-models are appropriate for addressing the computation issue of the MCS method. However, it should be noted that PCE showed significantly poor performance qualities when the new inputs with different inputs or probability ranges were used. This means that the PCE does not easily handle the various stochastic problems such as robust decision-making, retrofits, commissioning, and optimal design and control.

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