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Calibration and uncertainty analysis for computer models – A meta-model based approach for integrated building energy simulation

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HIGHLIGHTS

- We monitor and model an office building before, during and after an energy retrofit.
- We describe the advantages and the drawbacks of different calibration strategies.
- Piece-wise regression, Gaussian processes regression and model fitting techniques are used.
- We cross-validate the calibration comparing indicators obtained with different techniques.
- We present the calibrated prediction values for a reference meteorological year.

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ABSTRACT

In energy and environment field models are constructed, in general, based on well-defined physical phenomena and properties. Calibration and uncertainty analysis hold a particular interest because models represent a simplification of reality and, therefore, it is necessary to quantify to what degree they are imperfect before employing them in design, prediction and decision making processes. Integrated building energy models attempt to describe the effect of various internal and external actions (weather, occupancy, appliances, etc.) through physical relations (both algebraic and differential) and they are being widely used to design and operate high performance buildings, which are an essential component of a global energy strategy to reduce carbon emission and fossil sources depletion. An approach oriented to systems and able to integrate effectively field measured data and computer simulations for calibration in the modeling process has the potential to revolutionize the way buildings are designed and operated, and to stimulate also the development of new technologies and solutions in the field. The research presented in this paper aims to represent an initial step towards this integrated approach.

1. Introduction

The importance of uncertainty in energy modeling is often undervalued. A model represents a simplification of reality and therefore it is important to quantify to what degree it is imperfect before using it in design, prediction and decision-making processes. All these activities can receive a benefit from a meaningful and affordable representation of uncertainty. In energy and environment field, models are constructed based on well-defined physical phenomena and properties (e.g. energy balance, mass balance, conductivity, etc.).

At present, building energy performance simulation is a mature field and the growing level of detail of the available tools [1] results in a huge amount of parameters, all of which are uncertain to some degree. Although uncertainty can be easily estimated for many parameters, it is difficult to deal with it at the system level (aggregated effect of all uncertainties), in particular in building design process (design optimization performed before construction and commissioning) [2–13] and operational optimization (model predictive control and event detection in real time) [14–23].

High-performance buildings (both new and retrofitted) are an essential part of a global energy strategy to reduce carbon emission, fossil sources depletion and more in general, to obtain a reduced environmental impact in a cost-effective way. In order to achieve these results, it is required to rely heavily on validated models, both in the design and operational phase [1,20,24,25]. Far, since efficient buildings have to become a normal practice in a reduced time frame, due to the criticality of the global goals, it is necessary to foster the increase of field knowledge by focusing on the previously mentioned aspects. In other words, a "learning from performance" approach must be adopted to critically analyze the result of different design strategies and technologies.

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Nomenclature

Variables, parameters and statistical quantities

c	specific heat
d	observed/experimental data
E	electricity demand
f	weighting coefficient for intermittent operation
F	fuel demand
H	heat transfer coefficient
HC, CC	heating and cooling coefficient of the building
HS, CS	slope of temperature dependent heating and cooling energy demand
m	number of input variables, dimensionality of the input
n	number of experimental observations of the response, number of training points
Q	heat demand
T	temperature
x	input variables
X	input variables dataset
y	response variables
Y	response variables dataset
ε	random variable describing difference between predictions and observations
η	efficiency, gain utilization factor, losses utilization factor
θ	calibration inputs to the simulator, weight coefficients in the regression model
μ	mean value of variables
ρ	density
σ	standard deviation, hyperparameter
Σ	covariance matrix

Functions and operators

$G(\cdot)$	simulation model operator
$E(\cdot)$	expected value, conditional expectation
$cov(\cdot)$	covariance function
$f(\cdot)$	probability density and distribution function, function of likelihood
$g(\cdot)$	probability distribution for prior in Bayesian modeling
$h(\cdot)$	regression function
$k(\cdot,\cdot)$	kernel function (basis function)
$K(\cdot,\cdot)$	covariance function
$L(\cdot)$	likelihood function
$l(\cdot)$	log-likelihood function
$m(\cdot)$	mean function
$p(\cdot)$	probability density function

Subscripts and superscripts

$\bar{}$	average value of variable
*	test dataset
a	air
adj	adjusted
c	change-point
C	cooling
d	day
ext	external air temperature
f	weighting coefficient
gn	gains
H	heating
i, k	training value indexes
ind	temperature independent demand
ls	losses
n	noise (error)
set	set-point
sys	system
t	duration of the analysis period
tr	transmission
ve	ventilation

Modeling correctly uncertainty is time-consuming and requires an additional effort in the overall design and operational optimization phase but, on the other hand, can provide more robust design solutions [26–28] and decision-making processes [29,30].

For example, it is possible to obtain not only a deterministic solution to a problem but rather a probabilistic solution (probability distribution), thus helping to gain greater confidence in the results with respect to the propagation of errors and underlying complex interactions among factors.

As a matter of facts, accuracy of energy and environmental modeling is not the only problem involved in the process of creating high-performance buildings. Actually, other factors such as economy viability [31,32] and impact of climate change [33,34] are other problems that strongly influence the success or the failure of an investment [35–38] and, therefore, the repeatability of the related technical solution or design strategy within a certain context.

Building energy models attempt to describe through physical relations (both algebraic and differential) the effect of various internal and external actions (weather, occupancy, appliances, etc.). All these relations require the use of a large number of parameters and despite the fact that the results for each single component or sub-system can be easily validated, overall system simulation output can be far from the measured value [39] in real word applications. As a consequence, it is necessary to perform an uncertainty analysis procedure, in order to quantify properly how uncertainties in input reflect on output. This can be done, in general, by assigning appropriate statistical distribution to inputs, running several models (employing a sampling strategy) [24,36,40,41] and analyzing relevant statistics for selected outputs.

However, not all the aspects modeled have the same level of importance and not all the inputs give the same contribution to error propagation [42–44]. As a consequence, uncertainty analysis must be coupled with sensitivity analysis to attribute a measure to the relative importance of the different input parameters [2,41,45].

Further, a profound knowledge of the component (or process, or sub-system) level behaviour is itself fundamental but not sufficient, because it is also crucial to analyze, interpret and model complex interactions based on continuously updated field data [20,21,46], for example, in dynamic commissioning and monitoring of buildings [47], which require a multi-scale system analysis.

A modeling approach oriented to systems and able to integrate effectively field measured data, computer simulations and to address multiple scales and periods under uncertainty [48] has the potential to revolutionize the way buildings are designed and operated, and to stimulate also the development of new technologies and solutions. Improvement in building energy modeling can involve, in particular:

1. integration between model driven and data driven multi-objective design optimization;
2. characterization of the dynamics of multi-scale, multi-period energy systems;
3. control, prediction and event detection for energy systems.

There exists clearly a distinction between experimental data (i.e. gathered from experiments performed according to some predetermined strategy, they can derive from field measurements or computer experiments) and observational data (i.e. observations of a system which is not controlled for the experiment's sake) [41]. In general, only in existing buildings a limited amount of field data from the true physical system is available to inform about the unknown inputs and about the uncertainty associated with a simulation-based prediction. In this paper an existing building recently retrofitted and monitored is chosen as case study, because of the availability of field data for model calibration [49]. The practical aspects considered are:

1. uncertainty in observational data and predictions;
2. calibration by minimization of the discrepancy between the simulation model adopted and the actual physical system (simulated data and real observational data);
3. reduction of the complexity and computational effort for calibration and prediction.

Therefore, the scope of the research presented is identifying a general theoretical approach to the topic of uncertainty analysis and calibration of building energy simulation models. In this sense, the development of a complete and coherent methodology could provide the basis for robust optimization procedures in a model-based analysis of building (code compliance, certification, etc.) and for the creation of building energy meta-models [45] for predictive control and event detection. Besides that, the correct quantification of uncertainty can establish a convergent path with risk assessment procedures in efficiency and renewable energy projects, thus realizing a better connection and integration with techno-economic analysis field and forecasting the potential of efficiency and technological innovation.

2. Statistical formulation of model calibration problem

As highlighted before, energy research relies strongly on modeling techniques and the set of activities, which involve the quantification of uncertainty includes:

1. verification;
2. validation;
3. calibration;
4. uncertainty propagation.

The features of these different activities are reported in Table 1. The problem of calibration is related, first of all, with the creation of inverse models [6,50–52] from measured data through a supervised learning process [53–57]. Supervised learning is a form of inductive learning that creates a functional mapping from training inputs to observed outputs: given a set of training input vectors coupled with observed output, a supervised learning machine attempts to build a function that summarizes the input–output relationship. After that, in the calibration of detailed simulators, real data are used to make inference about simulator input starting from simulator output. In this sense, we use the functional mapping as a surrogate of the original model.

The research presented deals, in particular, with the calibration of models used in integrated building energy analysis, although the methodology can be applied to general computer models; the objective is to use observational data and simulator outputs to make inference about simulator inputs (unknown but bounded), as introduced before. In other words, the goal is to calibrate uncertain input parameters (both static and dynamic) to ensure that the model reproduces correctly the measured data, thus giving a validated representation of the physical phenomena under evaluation. The calibration procedure poses many practical problems, summarized in Table 2. In particular, this problem is ill-posed and could determine several possible matching models and, on the other hand, it is difficult to assess correctly modeling uncertainty starting from simulator outputs. Further, there are other specific tasks:

- model accurately multivariate input/output processes (multi-objective problems);
- enable multi-scale and multi-period data use;
- avoid error-prone modeling and computation;
- avoid a too intensive computation.

These tasks are added to the inherent complexity of the process. Several different types of models can be used for describing the energy behavior of a building [1,6,21,41,58] and all these models must be calibrated, depending on the specific application field [21]. A general categorization of model types is reported in Table 3. A simplified physically based model with unknown parameters optimized with respect to real data, a "grey-box" model, is more understandable than a "black-box" model (neural networks, support vectors machines, etc.) [41], however, a "black-box" model can achieve high accuracy with a fairly simple implementation, thus enabling multiple runs of the model with a reduced computational effort. Not all the parameters in this type of models are literally physical and transparent to the user [55,57] but, nonetheless, it must be recognized that, for the purpose of prediction, control and event detection, the direct use of "state of the art" building energy models ("white box" detailed models) poses several technical difficulties. In the subsequent paragraphs, the general mathematical formulation of the calibration problem and the essential tools employed are described.

Table 1
Quantification of uncertainty in modeling.

Activity	Description
Verification	Comparing computational and conceptual model to assess the errors introduced via numerical computation
Validation	Comparing computational model results with real outcomes (both experimental and observational data) to assess errors
Calibration	Comparing computational model with real outcomes with the objective of determining unknown (but bounded) variables in the model by minimization of the squared sum of the errors
Uncertainty propagation	Determining the uncertainty in model output with respect to uncertainty in input

Table 2
Problems in calibration procedure.

Problem	Description
Computational resources	Simulation can be computational intensive
Infeasibility of search	Exhaustive exploration of the parameter space can be infeasible
Multiple solutions	Various ranges and/or combinations of input variables may yield comparable fits to the observed data
Error in data	Observed data contain some degree of error or uncertainty
Multivariate input/output	Model response quantity of interest is multivariate (multiple objectives analysis, time-series analysis, etc.)
Agreement with observations	Agreement between given simulator output and biased and noisy observed/experimental data is not obvious nor trivial

Table 3
Different model types.

Model type	Description	Advantages	Disadvantages
White-box	Detailed mechanistic models or reference models based on the laws of physics that permit accurate modeling, employing algebraic and differential equations (ODE, PDE) to describe temporal and spatial variations	Accuracy and precision, detailed physical description of phenomena	Computational effort, difficult and error-prone modeling and implementation process
Grey-box	Models with a simplified description of the underlying physical phenomena in space and time with algebraic equations and first order ODE, available data are used to identify the best model, and to determine the model parameters.	Easier implementation with respect to white-box models, physical description of phenomena, computational efficiency	Not as accurate as accurate and precise as white-box models, error-prone implementation process
Black-box	Empirical or data-driven models are based on little or no physical behavior of the system and rely on the available data to identify the model structure. They are suitable for predicting future behavior under a similar set of conditions	Computational efficiency and flexibility, simple implementation with respect to the achievable accuracy	Absence of a physical representation, opaque to the user

2.1. General description of the calibration problem

First of all, we denote with $G(\cdot)$ the operator who represents a general computer model. This operator associates input variables to output variables. We denote with x the observable (in some cases controllable) inputs (i.e. explanatory variables) and with y the outputs (i.e. response variables). After that, we denote with θ the values of additional unobservable input variables and tuning parameters, which are required to obtain a calibrated computer model. Although there is clearly a distinction between calibration variables (physical quantities) and tuning parameters (purely numeric quantities, dependent on the specific computational technique chosen), we will take the term calibration to include both types throughout this paper and the methods presented will have to deal with both, although from a different point of view in the computational process. Therefore, in general models, it is possible to consider variables associated with calibration and parameters associated with algorithms tuning, indicated later as hyperparameters [56]. In other words, we calibrate the model with respect to both input variables and model parameters (numeric model refinement) but dealing with them separately from a conceptual point of view. We can express a general computer model with the following expression:

$$y = G(\theta, x) \tag{1}$$

Now we consider a set of n experimental or observational measures, according to definition introduced previously, and we denote it with d where:

$$d = d_1, \ \ldots \ , d_n \tag{2}$$

We introduce the notation ε_i for a random variable describing the difference between model predictions y and observations d_i, thus obtaining the following expression:

$$d_i = G(\theta, x) + \varepsilon_i \tag{3}$$

Various statistical methods can be used for the calibration of computer simulations [59–62] and one of the most straightforward ways is performing a non-linear regression analysis with respect to the observational data and the computational model output. In this case, the problem is solved using optimization techniques to minimize the sum of the squares of the residuals between model predictions and observed/experimental data. The root of the squared mean of the residuals between the experiments and the predictions is defined as:

$$\mathrm{RMS} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(d_i - G(\theta, x_i))^2} \tag{4}$$

This approach can be useful for an initial deterministic estimation of the calibration variables and parameters and can lead to a first estimation of them (direct model fitting) with a limited number of runs (underlying computer model runs) of the nonlinear regression objective function (RMS). Although intuitive in the formulation, this approach presents several drawbacks, summarized in Table 4.

With respect to the last aspect, it is possible to estimate the uncertainty of solution by using simulation–optimization techniques [63] and choosing sampling strategies (i.e. Monte Carlo, Latin Hypercube, etc.) [36]. This, of course, will require a much larger number of model runs and will, consequently, increase the magnitude and the impact of the problems described in Table 4.

From a practical point of view, it makes more sense to use an approximation of the model to perform this analysis (meta-model or reduced order model) [64] constructed following a supervised learning approach. In supervised learning, training and testing data (observational input/output data) to construct a predictor, as illustrated in Fig. 1. A predictor can be a classifier (discrete values) or a regressor (continuous values).

The method will be described in detail in Section 2.3. With a reduced-order model uncertainty analysis is easier to perform than with a detailed simulation model, because the mathematical formulation of the model is far more simple than the original one (linear/polynomial multivariate regression, kernel regression, neural networks, etc.). A comprehensive treatment of the uncertainties in the modeling process can be achieved with Bayesian analysis, introduced in the next section.

2.2. Bayesian analysis and calibration framework

Bayesian analysis [56,57,65,66] is a statistical inference method in which unknown variables (e.g. input variables/parameters in model calibration) are treated like random variables. In this way, probability theory can be applied not for finding "best-fit" models, but rather to compute a posterior probability distribution for new data (e.g. for the output of a regressor). First of all, a probability "prior" distribution function is assigned to the model uncertain

Table 4
Problems in direct model calibration with RMSE minimization.

Problem	Description
Computational effort	Depending on model characteristics, finding the set of calibration variables and parameters that minimizes RMS can be costly (large number of model runs) and even infeasible
Multiplicity of solutions	Depending on the formulation of the model, there can exist various calibration variables and parameters ranges that provide similar values for the objective function RMS (problem of uniqueness of solution), thus determining an additional difficulty with respect to the selection of the appropriate values, and there can be numeric instability in the solution (ill-defined optimization problem)
Deterministic solution	Only one deterministic solution is found, it is not possible to evaluate the uncertainty associated with that solution if we are employing biased and noisy data

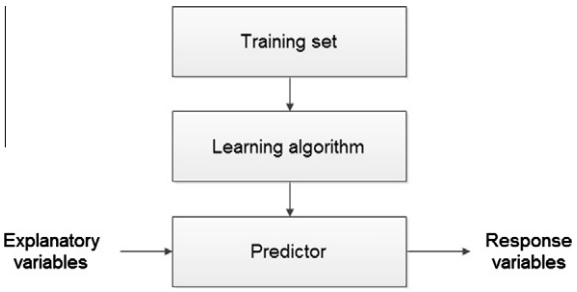

Fig. 1. Scheme of the process of supervised learning.

inputs and then the distribution functions are refined based on available data, so that the resulting "posterior" distributions represent the new state of knowledge, based on observed/experimental data characteristics (substantially a prediction). Despite the computational effort, this method provides a complete description of uncertainty valuable, for example, for robust prediction and stochastic optimization, requiring an intensive computation [66]. The Bayesian analysis is based on Bayes rule, which states that:

$$f(\theta|d) = \frac{g(\theta)f(d|\theta)}{\int_{\theta' \in \Theta} g(\theta')f(d|\theta')d\theta'} \tag{5}$$

where θ is the vector of unknown inputs; Θ is the domain of function $g(\theta)$; d are the observations; $g(\theta)$ is the prior probability; $f(d|\theta)$ is the likelihood; $f(\theta|d)$ is the posterior probability.

Or in a simpler way:

$$\text{posterior} = \frac{\text{prior} \times \text{likelihood}}{\text{marginal likelihood}} \tag{6}$$

Since d values (observations/experimental data) are fixed, likelihood is indicated in general with $L(\theta)$ instead of $f(d|\theta)$. From Eq. (5) we derive the following:

$$f(\theta|d) \propto g(\theta)L(\theta) \tag{7}$$

In statistical estimation the specific task is maximizing the likelihood function $L(\theta)$, in order to obtain robust models. The most frequently used assumption for the ε_i in Eq. (2) is that they are independent and identically distributed (i.i.d.) Gaussian with 0 mean and variance σ^2 (white noise):

$$f(d|\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(\varepsilon_i)^2}{2\sigma^2}\right] \tag{8}$$

By substituting expression (3) in (8) we obtain the following:

$$L(\theta) = f(d|\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(d_i - G(\theta, x_i))^2}{2\sigma^2}\right] \tag{9}$$

The maximization of the previous function is equivalent to the maximization of the log-likelihood function which is easier to handle from a mathematical point of view:

$$l(\theta) = -\left(\frac{n}{2}\right)\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}[(d_i - G(\theta, x_i))^2] \tag{10}$$

The posterior distribution $f(\theta|d)$ represents the complete state of knowledge for model output. By knowing the posterior distribution we can calculate fundamental statistics such as the mean, the standard deviation (or the variance) and others. Similarly to the general case with RMS minimization, reported in Eq. (4), when the posterior distribution cannot be constructed analytically[1] it is necessary to use sampling techniques [66] and, therefore, multiple model runs are necessary (output data obtained from multiple model runs can be fitted to a distribution to provide a synthetic description). Another way to solve the problem of likelihood maximization is to use the marginal likelihood, denominator of expression (5), This approximation in known as type II maximum likelihood [5] and it is applied in Gaussian processes parameters tuning.

[1] If $G(\theta, x)$ is a linear model where ε follows a Gaussian distribution with 0 mean and σ^2 variance it is possible to prove that Eq. (8) reduces to least square minimization problem.

2.3. Linear regression, Bayesian regression and Gaussian processes regression

In this section, the use of supervised learning for regression is described. The simplest form of regression is linear regression which we can introduce with the following expression:

$$h(x) = \sum_{i=0}^{m} \theta_i x_i = \theta^T x \tag{11}$$

In the previous expression we assume the notational convention that $x_0 = 1$, this is the intercept term, and m is the number of input variables (not counting x_0).

To derive θ, we will define a function that measures, for each value of θ, how close the $h(x_i)$ values are to the corresponding y_i (observational data). This is expressed as:

$$J(\theta) = \sum_{i=1}^{n} (h(x_i) - y_i)^2 \tag{12}$$

$J(\theta)$ (cost function) is minimized by:

$$\theta = (X^T X)^{-1} X^T y \tag{13}$$

where X is the matrix with training input data (made by x vectors); y is the vector with training output.

The previous expression is the analytical solution (first-order derivative equal to zero) of least squares minimization problem (using linear algebra) and represents the basis for the supervised learning presented in Fig. 1. The goodness of fit can be verified by analyzing RMSE, introduced in Eq. (4), and R^2 which is defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y - y_i)^2}{\sum_{i=1}^{n}(y - \bar{y})^2} \tag{14}$$

In general, it is necessary to analyze also the distribution of the residuals, in order to demonstrate that they are i.i.d., and verify significance with test T and test F [67]. From a probabilistic point of view, linear regression can be expressed with:

$$y_i = \theta^T x_i + \varepsilon_i \tag{15}$$

Linear regression framework can be extended for example by:

- using basis expansions, such as $x_2 = x_1^2, x_3 = x_1^3$ leading to a polynomial representation;
- establishing relations/interaction between variables $x_3 = x_1 x_2$;
- using functions which are linear in their parameters (generalized linear models);
- using kernel functions (according to Mercer's condition for kernel).

For a distinction between linear models which are linear, non-linear/linear in the parameters and non-linear in both model and parameters refer to [41]. In the latter case it is necessary to solve a non-linear least squares problem such as the one depicted in Eq. (4) while, if we exploit the properties of the "extended" linear regression framework, we can obtain efficient "black-box" meta-models (inverse models created from data), no matter the origin of our x_i, provided that the basis function chosen are linear in the

parameters and satisfy Mercer's condition for kernels (i.e. positive semidefinite covariance matrix) [55,56]. Further, due to the specific characteristic of the computer model calibration problem, a Bayesian analysis methodology is necessary to address uncertainty both in input and output (probabilistic modeling). For this reason Gaussian Processes (GP) regression technique with kernel functions was chosen to create the meta-models. GP regression, while remaining in the Bayesian framework, brings many advantages that will be illustrated subsequently and enable the analytical solution of likelihood maximization without requiring a sampling strategy and several model runs (required in general for Bayesian analysis). The basic idea of the GP model is that the response values y are modeled as a group of multivariate normal random variables. The multivariate Gaussian is defined as:

$$p(x;\mu,\Sigma)=\frac{1}{(2\Pi)^{m/2}|\Sigma|^{1/2}}\exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right) \tag{16}$$

where x is a vector valued random variable; m is the number of input variables (dimensionality of input); μ is the mean of the distribution; Σ is the covariance matrix; $|\Sigma|$ is the determinant of covariance matrix.

In a compact notation:

$$x\sim N(\mu,\Sigma) \tag{17}$$

Gaussian distribution is extremely common when modeling error ("noise") in statistics and is convenient for analytical manipulations. The useful properties of the multivariate Gaussian are normalization, marginalization, conditioning and summation [56]. We define a GP model with mean function $m(\cdot)$, covariance function $k(\cdot,\cdot)$, with $x_1,\ldots,x_n\in X$ and the associated values $h(x_1),\ldots,h(x_n)$ with the following notation:

$$\begin{bmatrix}h(x_1)\\ \vdots\\ h(x_n)\end{bmatrix}\sim N\left(\begin{bmatrix}m(x_1)\\ \vdots\\ m(x_n)\end{bmatrix},\begin{bmatrix}k(x_1,x_1) & \ldots & k(x_1,x_m)\\ \vdots & \ddots & \vdots\\ k(x_m,x_1) & \cdots & k(x_m,x_m)\end{bmatrix}\right) \tag{18}$$

In a compact form we can write:

$$\begin{aligned}&h(\cdot)\sim GP(m(\cdot),k(\cdot,\cdot))\\ &m(x)=E[x]\\ &k(x,x')=E(x-m(x))(x'-m(x'))\end{aligned} \tag{19}$$

We can introduce, exploiting the property of summation of multivariate Gaussians, a "white noise" zero mean Gaussian error with σ^2. The error is defined with the following notation:

$$[\varepsilon]\sim N(0,\sigma^2) \tag{20}$$

This passage extends the possibility of application of Gaussian processes to realistic problems with data affected by uncertainty. We define the covariance function (in matrix notation) for a problem with noisy observations as:

$$cov(y)=K(X,X)+\sigma^2 I \tag{21}$$

The use of GP for prediction (i.e. supervised learning) implies the application on new data of the meta-model trained and tested on available observed/simulated data affected by a Gaussian error. If we denote with X and y the training dataset (input and response) and X_* and y_* the test dataset, we obtain that:

$$\begin{aligned}&\begin{bmatrix}y\\ y_*\end{bmatrix}\Big|X,X_*\sim N(m(x),cov(y))\\ &m(x)=K(X_*,X)(K(X,X)+\sigma^2 I)^{-1}y\\ &cov(y)=(K(X_*,X_*)+\sigma^2 I)-K(X_*,X)(K(X,X)+\sigma^2 I)^{-1}K(X,X_*)\end{aligned} \tag{22}$$

These equations can be interpreted as a linear combination of n kernel functions (despite the fact that the GP can be represented in terms of a possibly infinite number of basis functions), each one centered on a training point, by writing:

$$\begin{aligned}&y=\sum_{i=1}^{n}\alpha_i k(x_i,x_*)\\ &\alpha_i=(k(X,X)+\sigma^2 I)^{-1}y_i\end{aligned} \tag{23}$$

The possible kernels to be used in the formulation are all the ones giving origin to a positive semidefinite covariance matrix. Three possible kernel functions are the following ones:

$$\text{polynomial}\quad k(x,x')=(1+(x,x'))^d \tag{24}$$

$$\text{radial basis}\quad k(x,x')=\exp\left(-\frac{1}{2\tau^2}\|x-x'\|^2\right) \tag{25}$$

$$\text{sigmoid}\quad k(x,x')=\tanh(k_1(x,x')+k_2) \tag{26}$$

The parameters which define the kernel functions in expression (23) are called hyperparameters (algorithm tuning parameters) [56], and they can be varied to fine-tune the meta-model. In the case of a multivariate radial basis kernel, used in several practical applications [55,56,68], we obtain the following:

$$k(x,x')=\sigma_f^2\exp\left(-\frac{1}{2}(x-x')^T M(x-x')\right)+\sigma_n^2 I \tag{27}$$

In this case $M=\tau^{-2}I$ and τ is a vector of positive values and parameter σ_f is introduced to weight the different kernels. The three main reasons for the choice of GP model for realistic modeling problems (i.e. with noisy observations) are:

- the possibility of choosing different types of kernel (in order to appropriately exploit data structure);
- the possibility of using a simple linear algebra implementation (and varying hyperparameters to adapt the model with a sensitivity analysis);
- the possibility of tuning hyperparameters via marginal likelihood maximization (solvable with gradient based methods).

In general, GP regression method is a well-known technique for the analysis of data from both physical phenomena and computer experiments'. Further, the ability to handle problems with highly multivariate input/output allows the use of this technique also for problems with multiple time and space variables, like real-time building energy simulation and model predictive control [69,70]. In any case, the peculiarity of this technique is that we obtain both an average (expected) value and a confidence interval, thus enabling a clear indication of the uncertainty level of our prediction.

2.4. Model selection and feature selection problem

Model selection is related to the evaluation of possible different models for a supervised learning problem. An important subset of model selection is feature selection. Feature selection involves the selection of subsets of relevant features from large datasets with many potential benefits like:

- facilitating data visualization and data understanding;
- reducing the measurement and storage requirements;
- reducing training and utilization times;
- defying the curse of dimensionality while maintaining adequate prediction performance.

The core problem is constructing and selecting subsets of features (fundamental input variables, to reduce model size via reduced-order models) that are useful to build a good predictor (i.e. best fit meta-modeling technique). These goals are generally conflicting because selecting the most relevant variables and therefore reducing the size of the training dataset is usually suboptimal for building a predictor [71,72]. Feature selection is performed first, according to criteria that will be illustrated hereafter, and then it is necessary to compare the results obtained with different learning algorithms [73]. If our purpose is constructing a predictor (e.g. a regression model for prediction), the general methodology to be followed is described in Fig. 2. Many feature selection algorithms include variable ranking as a principal selection mechanism because of three main reasons:

- simplicity;
- scalability;
- good empirical success.

Variable ranking is a filter method (pre-processing step), independent of the choice of the predictor [71]. Still, under certain independence orthogonality assumptions, it may be optimal with respect to a given predictor [53]. The selection of features is done by taking into consideration ranking criteria (i.e. sensitivity of some suitable index). Two possible ranking criteria are depicted: correlation criteria and information theoretic ranking criteria. Correlation criterion is based on Pearson's coefficient calculated according to the following:

$$R(i) = \frac{cov(X_i, Y)}{\sqrt{\mathrm{var}(X_i)\mathrm{var}(Y)}} \tag{28}$$

where *cov* indicated the covariance and var the variance. The estimate of $R(i)$ is given by:

$$R(i) = \frac{\sum_{k=1}^{n}(X_{k,i} - \overline{X}_i)(y_k - \bar{y})}{\sqrt{\sum_{k=1}^{n}(X_{k,i} - \overline{X}_i)^2 \sum_{k=1}^{n}(y_k - \bar{y})^2}} \tag{29}$$

The information theoretic ranking criterion $I(i)$ is a measure of dependency between the probability density of variable x_i and the probability density of the target y is expressed by:

$$I(i) = \int_{x_i}\int_{y} p(x_i, y) \log \frac{p(x_i, y)}{p(x_i)p(y)} dx\, dy \tag{30}$$

where $p(x_i)$ and $p(y)$ are the probability densities of x_i and y; $p(x_i, y)$ is the joint density of x_i and y.

For discrete nominal variables the expression becomes:

$$I(i) = \sum_{x_i}\sum_{y} P(X = x_i, Y = y) \log \frac{P(X = x_i, Y = y)}{P(X = x_i)P(Y = y)} \tag{31}$$

The densities $p(x_i)$, $p(y)$ and $p(x_i, y)$ are unknown and hard to estimate from data for the continuous case. It is much easier to use discrete nominal variables because the probability densities are estimated from frequency counts. Recent developments of this technique enable knowledge extraction from large datasets in several different fields of application [74].

3. A case study of building energy model calibration

The case study presented is the calibration of the energy simulation model of an office building which has been retrofitted in recent years. In Fig. 3 the pictures of the building before retrofit, after retrofit and the computer model are reported. This building has been monitored before, during and after the intervention, following the subsequent steps:

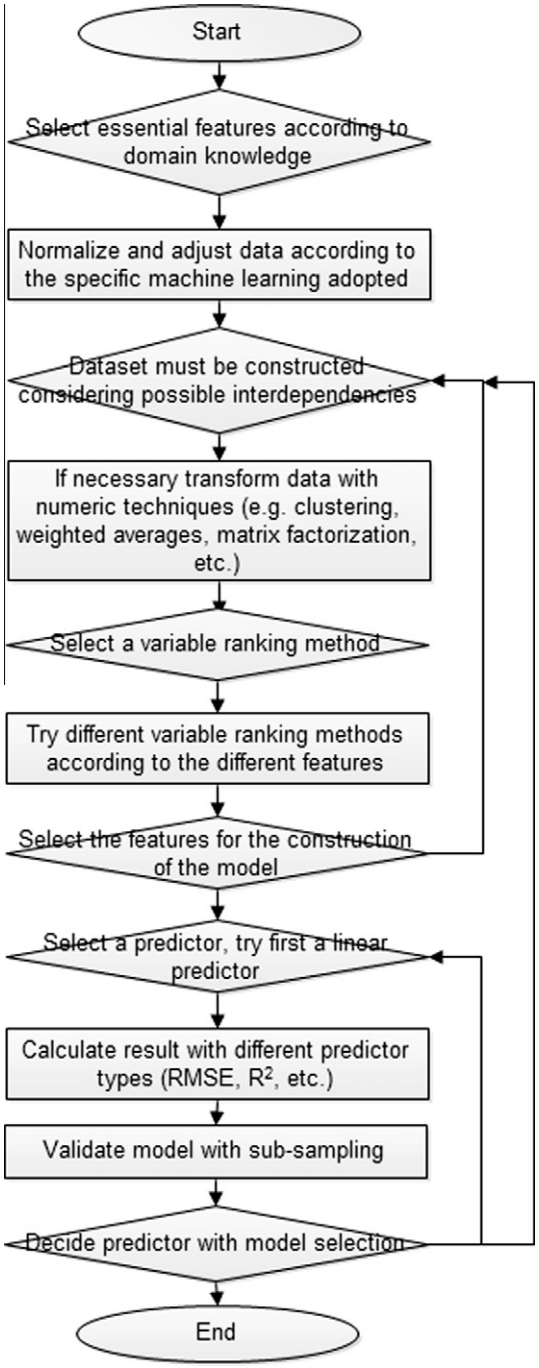

Fig. 2. Flow chart of the feature and model selection process.

1. measuring energy use and influential variables before, during and after the retrofit;
2. calculating normalized energy consumption for the period before and after retrofit, with respect to a typical meteorological year;
3. constructing a calibrated simulation model for the operational optimization in the period after retrofit and the analysis of possible further interventions.

The first two steps are suggested by ASHRAE guidelines for measuring retrofit savings [51,52,75] and were performed to verify them during building operation. After that, calibrated simulation models have been created for providing a useful representation

of building energy behavior. Several computational tools have been used, but uncertainty in the assumptions was not taken into account explicitly in the initial phase (i.e. by formulating a probabilistic model). The calibration of the detailed simulation model was computationally intensive and so it was worth studying a strategy to reduce the overall complexity. The key points of the research are the following ones:

1. verify energy saving measures effect;
2. create a validated building model for baseline analysis design of other possible intervention (design optimization);
3. verify and manage control strategies in the operational phase (HVAC control, energy management);
4. verify experimentally the accuracy of the simulation models generally adopted in building energy design.

The methodology employs different models and, for each one, it is necessary to define a structure with input variables (explanatory variables) and output variables (response variables). In probabilistic modeling, outputs are probability distributions to be confronted with real measured data. The overall process is based on the following steps:

1. data collection (measurement);
2. model creation (hypothesis);
3. model calibration (synthesis).

3.1. Inverse modeling for normalization of energy consumption and direct model calibration

As introduced before, the first step for the analysis of energy consumption is discriminating temperature dependent (heating/cooling) and temperature independent natural gas and electricity demand (appliances, lighting). The method adopted is described both by ASHRAE and EN 15603 norm and is called "energy signature" model. The core assumptions of this method are:

- stable internal operating conditions (controlled internal environmental conditions);
- stable internal gains;
- low passive solar gains;
- external temperature as the most influential parameter.

It represents a rough but very useful description of building energy behavior where, first of all, we create a scatter-plot of energy consumption with respect to external temperature for different periods. After that, a piece-wise regression model is fitted on real data. Similarly, the detailed simulation model for the period after retrofit is calibrated in a direct way by RMSE minimization. In the first case the problem is solved using gradient method, in the second case using heuristics. Monitoring involves the following periods:

- before retrofit (2004–2007);
- during retrofit (2008–2009);
- after retrofit (2010-present).

The values of RMSE and R^2 obtained with the piece-wise regression model are reported in Table 5. Residuals, if the model is constructed correctly, must assume (approximately) a Gaussian distribution which tells us that errors in the model are fundamentally uncorrelated (i.i.d.); in both cases the distribution of residuals confirms this assumption. In Figs. 4 and 5 electricity and natural gas average hourly demands are represented as a function of average daily external temperature for the different periods, while in Fig. 6 temperature dependent electricity demand (cooling) and natural gas demand are represented for the different monitoring periods along with the data obtained with the calibrated detailed simulation for the period after retrofit. Finally, in Fig. 7 electricity for cooling and natural gas for heating are represented for the different months in the period after retrofit, along with the data obtained with the piecewise regression and the detailed simulation, highlighting the difficulty of creating a detailed deterministic model matching real observational data.

In this phase, it is possible to cross-validate the results obtained with the two different modeling strategies, taking into account the differences. We need to consider the following expressions [51,75]:

$$E = E_i + CS(T_{a,ext} - T_{c,C}) \tag{32}$$

$$F = F_i + HS(T_{c,H} - T_{a,ext}) \tag{33}$$

$$T_{c,C} = T_{a,set} - \frac{Q_{gn,\mathrm{day}}}{CCt_{\mathrm{day}}} \tag{34}$$

$$T_{c,H} = T_{a,set} - \frac{Q_{gn,\mathrm{day}}}{HCt_{\mathrm{day}}} \tag{35}$$

$$CC = H_{tr} + f_C H_{ve} \tag{36}$$

$$HC = H_{tr} + f_H H_{ve} \tag{37}$$

$$CS = \frac{CC}{\eta_{sys,C}} \tag{38}$$

Fig. 3. Picture of the building before retrofit, after retrofit and the simulation model.

Table 5
RMSE e R^2 of piece-wise regression models for the different periods.

Period	Inverse models		R^2
	demand	RMSE	
Before retrofit (2004–2007)	Electricity (kWh)	15.1	0.85
	Natural gas (m^3)	3.0	0.88
During retrofit (2008–2009)	Electricity (kWh)	12.1	0.73
	Natural gas (m^3)	1.9	0.94
After retrofit (2010-present)	Electricity (kWh)	6.4	0.90
	Natural gas (m^3)	2.3	0.90

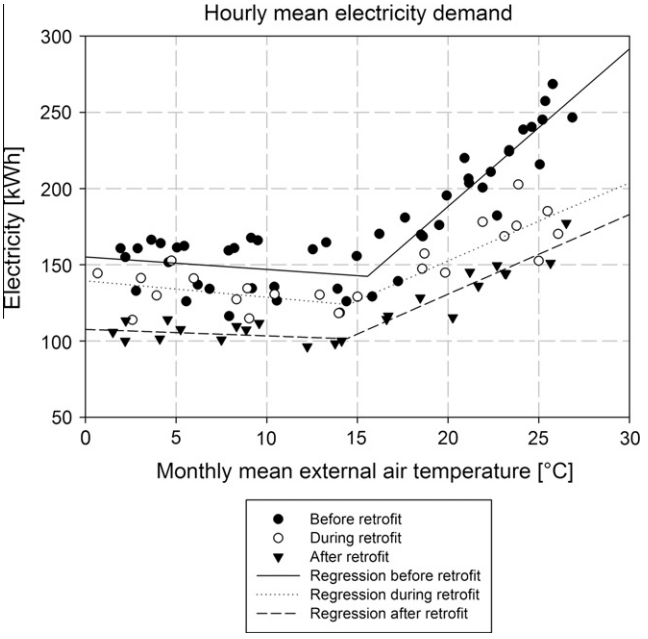

Fig. 4. Hourly mean electricity demand in the different monitoring periods and piece-wise regression models.

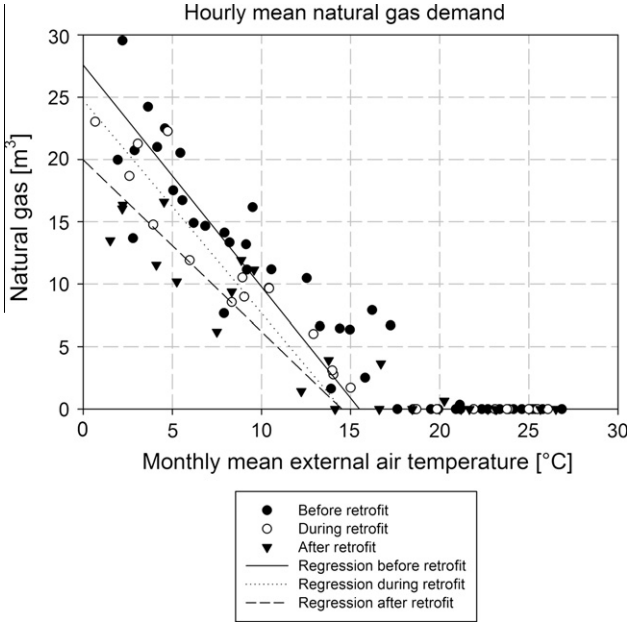

Fig. 5. Hourly mean natural gas demand in the different monitoring periods and piece-wise regression models.

$$HS = \frac{HC}{\eta_{sys,H}} \tag{39}$$

By employing these relations we can evaluate with the two different models *CC*, *CS*, *HC* and *HS*. The agreement between results obtained with the two different models is presented in Table 6.

3.2. Meta-model construction and variables definition

In the construction of a meta-model it is necessary to standardize and to categorize the different input and output variables and to construct a dataset accordingly. This, of course, represents clearly a simplification, because the variables chosen can be themselves synthetic indicators whose aim is to represent, without losing too much accuracy, a larger set of variables (e.g. weighted averages, standard reference values, etc.). This happen in particular with values collected as time series those must be expressed by a synthetic representative value (i.e. indicator). The variables are organized in the following groups:

1. climatic conditions and location;
2. envelope;
3. activities;
4. lighting;
5. control and operation;
6. water loop;
7. air loop;
8. air handling units;
9. terminal units;
10. domestic hot water (DHW);
11. distributed generation.

The detailed variables list is reported in Table 7 for the different groups. In Table 8 a summary of the values for the case study is presented.

Occupancy, plug load and artificial lighting load have been modeled starting from data collected in a survey (in situ measurements) for the case study.

In synthesis, average occupancy profile's multipliers have been considered, rescaling the overall profile considered in the simulation by substituting the peak value (i.e. the profiles maintain the same shape but can vary within certain boundaries so that it reproduces the more plausible profile).

In this sense, we have to embrace a stochastic dynamic modeling perspective. In fact, as highlighted in many recent researches on occupancy forecasting, different strategies are possible, namely sensor-utility-networks [76,77], agent based and graphical models [78,79] and fusion of heterogeneous data [80,81].

Although from a different perspective, they all employ techniques such as Kalman filter (KF), Hidden Markov Model (HMM) and, more in general, Bayesian analysis.

Despite some differences in the assumptions and in the calculation (e.g. hidden state variables are continuous in KF and discrete in HMM, KF assumes a Gaussian noise while HMM can represent arbitrary state distributions, etc.) a "unified" vision of these techniques is possible [82].

With respect to this data structure, the most influencing variables have been identified based on a data analysis process, illustrated in the next section. However, it was important first of all to identify the fundamental components considered in the modeling process.

3.3. Feature selection for model reduction and Gaussian processes meta-model training

In our case study, the most influential variables are the ones related with the behavior of the building envelope (transmittance,

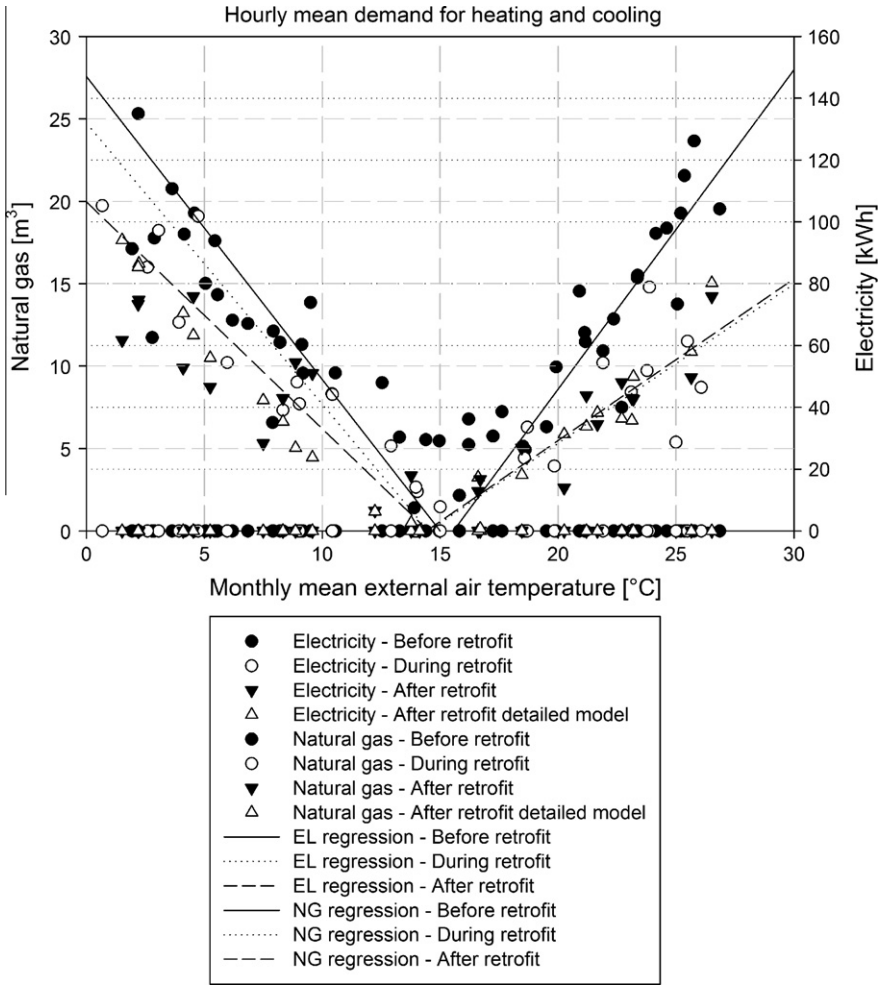

Fig. 6. Hourly mean electricity and natural gas demand for cooling and heating in the periods before, during and after retrofit and the values obtained with the calibrated simulation model for the period after retrofit.

thermal capacity and shading control system) and the ones related with operating schedules and set-points of HVAC system.

In order to account for the possible variations in the input for the detailed model, many simulations are run for the typical meteorological year according to a three levels Design of Experiment (DOE) strategy [83,84]. Lower bound, upper bound and mean values are considered for every uncertain input variable, thus giving origin to several possible combinations (i.e. model runs). After that a dataset with explanatory and response variable is constructed from the computer experimental data generated based on the logical structure defined in the previous section. As introduced before, in our case study, explanatory variables are the ones related with building envelope and solar shading control system, because they are difficult to measure directly (other uncertain variables have been directly measured in the monitoring process), while response variables are electricity demand for cooling and natural gas demand for heating. The GP meta-model is trained on simulated data, using a radial basis kernel function and adjusting hyperparameters.

Using the GP meta-model created it is possible to infer about model input based on model output and, consequently, to determine the input variables (explanatory) that return the selected output variables (response). Output variables are normalized (for a typical meteorological year) electricity for cooling and natural gas for heating. Therefore, we the piece-wise regression data are the basis for meta-model based calibration. The calculated input variables can then be substituted back in the detailed simulation model, in order to obtain the calibrated simulation model.

In the next section, the prediction values (normalized electricity and natural gas demand) for a typical meteorological year are presented for the following cases:

1. piece-wise regression;
2. detailed simulation calibrated through GP meta-model;
3. detailed simulation calibrated directly by RMSE minimization.

In a general case, a complete dataset can be constructed based on the structure proposed in Table 7. By performing feature selection, explanatory variables can be ranked based on their importance (i.e. the input variables that affect the output most obtain a higher score). In this way, feature selection can be effectively applied directly to data before training a meta-model, to obtain a reduced-order model (by eliminating redundant variables). This is useful both for model calibration (definition of the correct input variables for a detailed simulation model) and for design optimization (several possible configurations are generated with computer experiments, and then optimization is performed on a reduced-order meta-model), reducing computational effort. Coupling DOE with meta-models can reduce the difficulties related to the direct use of optimizers on detailed models, with a better exploitation of the current possibilities given by supervised learning and optimization algorithms [10]. Further, meta-models can be employed for uncertainty and sensitivity analysis, increasingly important topics in high efficiency buildings [2,45], in a much easier way than detailed simulation models: although there exist other strategies

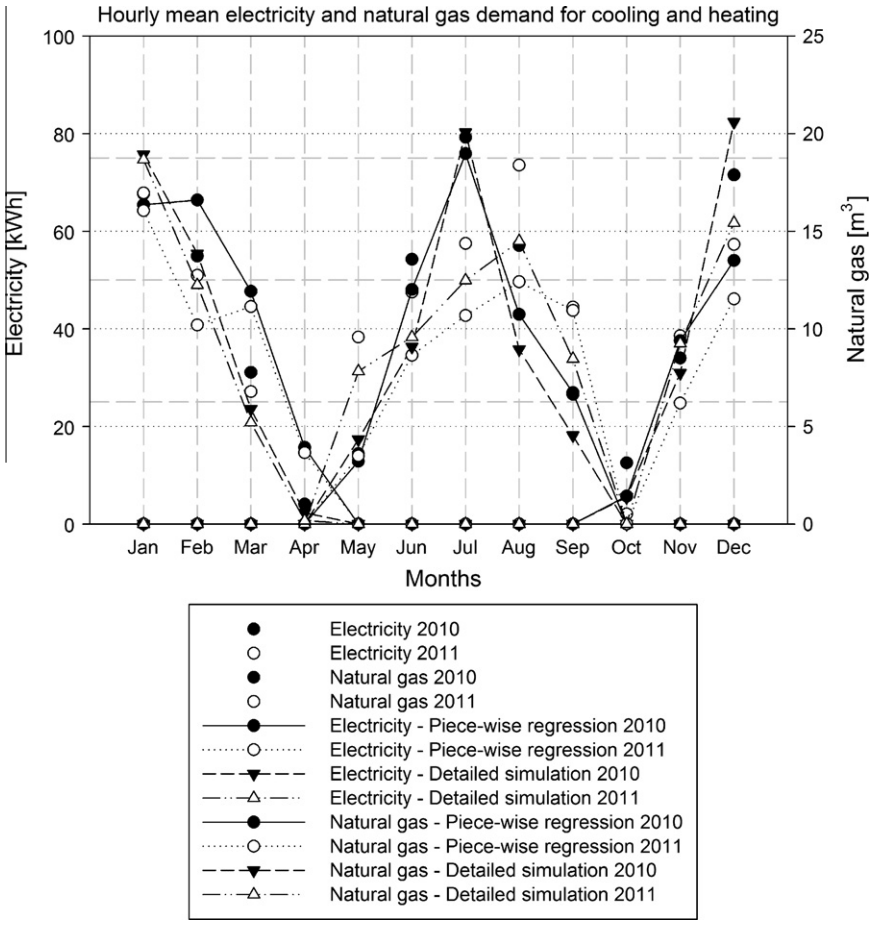

Fig. 7. Hourly mean electricity and natural gas demand for cooling and heating in the period after retrofit fitted with piece-wise regression and detailed simulation.

Table 6
Parameters for the cross-validation of inverse modeling and calibrated simulation.

Model	*HC* (kWh/K)	*CC* (kWh/K)
Piece-wise regression model	8541.0	12930.1
Detailed simulation model	8349.6	13161.1

for addressing these issues, the methodology presented seems the most promising.

3.4. Comparison of results from different models and calibration through meta-model

In this section the values obtained with the simple inverse model (piece-wise regression), the meta-model (Gaussian processes regression) and the detailed calibrated simulation model are presented. The reduced-order meta-model, as described earlier, is trained based on computer experimental data. After that, the meta-model is used for calibrating input variables (explanatory variables) with respect to normalized observed data (output). Of course, the direct calibration of meta-models with real observed data (similarly to the case of the detailed simulation model for the period after retrofit) could give more accurate results, but, in order to simplify as much as possible the process for reproducibility, we decided to simply integrate piece-wise regression model (useful in the first assessment phase) trained on real data and computer generated experimental data (required for the construction of the detailed simulation model). The results obtained are reported in Fig. 8 and Table 9, enabling a rapid comparison of the accuracy achievable with the different approaches. The different models nearly matches for the yearly heating energy consumption of natural gas, while for the estimated yearly electricity consumption for cooling there is a 4.7% relative difference between the lower and the higher value. In any case, the approach proved to be valuable for the empirical estimation of the global heat exchange coefficient of the building, as highlighted in Section 3.1, as well as other variables in detailed modeling. Additionally, despite the computational effort required by DOE and meta-modeling, the advantages of having a full spectrum of detailed models' results are indubitable. The meta-models trained on this data offer several advantages with respect to the detailed ones in term of usability and computational speed in optimization, uncertainty and sensitivity analysis [85] with a comparable level of accuracy. Further, sensitivity analysis can be performed automatically in large datasets by using feature selection to identify the most influential variables. Finally, this technique can become particularly useful for buildings with detailed automatic data acquisition, in which computer generated data have to be confronted with field observational data.

4. Conclusions

The importance of computational models in design, prediction and decision making processes determines the necessity of appropriate methods for assessing the robustness of the results. This paper describes a methodology for calibration and uncertainty analysis of building simulation models, applied to a monitored building case study. In this case study the practical problems to

Table 7
Variables for detailed energy modeling.

Group	Variables
Climatic conditions and location	Climatic dataset (temperature, relative humidity, solar radiation, etc.)
	Design days (winter, summer)
Envelope	Building geometry (dimension)
	Building construction (walls, roofs, basement, etc.)
	Building shading system
Activities	Appliances, process, occupancy (gains, schedules, etc.)
Lighting	Lighting (installed power, schedules, control system, etc.)
Control and operation	Set-points (temperature, humidity and schedule)
	Ventilation (minimal outdoor ventilation rate, minimal mechanical ventilation rate, maximal mechanical ventilation rate)
	Heating/cooling (minimum/maximum outdoor temperature for operation, minimum/maximum hot water and chilled water temperature)
	Shading control system
Water loop	Pumps (rated head, flow rate efficiency, loss fraction, specific power)
	Water pipes (length, insulation)
Air loop	Fans (pressure rise, flow rate, efficiency, loss fraction, specific power)
	Air ducts (length, insulation)
Air handling units (AHUs)	Temperatures of fluids (chilled water inlet/outlet temperatures, hot water inlet/outlet temperatures)
	Humidification (adiabatic humidifier effectiveness, humidifier efficiency)
	Fans (pressure rise, flow rate, efficiency, loss fraction, specific power)
	Pumps (efficiency)
Terminal units	Heating/cooling average emission temperature
	Heating/cooling average emission efficiency
	Heating/cooling terminal units COP
Domestic hot water (DHW)	Number of occupants, type of end use
Plant	Heating generation (efficiency, COP, fuel, etc.)
	Cooling generation (EER, fuel, etc.)
	Condenser/evaporator (ranges of temperature, flow rate)
	Cooling tower (range of temperature, fans, etc.)
Distributed generation	Generation technology (installed capacity, conversion efficiencies, fuel type, etc.)

Table 8
Summary of variables for the case study.

Group	Type	Unit	Value
Climatic conditions and location	Latitude and longitude	°	45°28′N, 9°10′E
	Heating/cooling design temperature	°C	−5/32
Envelope	Number of building blocks	–	3
	Net floor area	m^2	5236
	Net volume	m^3	18,355
	External walls *U* value	W/(m^2 K)	0.36
	Roof *U* value	W/(m^2 K)	0.38
	Basement *U* value	W/(m^2 K)	0.54
	Transparent surfaces *U* value	W/(m^2 K)	1.7
	Transparent surfaces *g* value	–	0.68
Activities and lighting	Total internal loads (average)	W/m^2	17.1
Control and operation	Heating set-point	°C/%	21/50
	Cooling set-point	°C/%	26/50
	Design ventilation rate (CAV)	m^3/h	45,000
	Minimum ventilation rate external air (IAQ)	m^3/h	30,000
AHU	Number of AHUs	–	3
Plant	Heating plant efficiency	–	0.59
	Cooling plant EER	–	2.27

be solved were, on the one hand, the verification and control of energy saving measures results and, on the other hand, the construction of a validated building simulation model for operational optimization and design optimization of further interventions (HVAC system retrofit and DG technologies adoption).

Three models were adopted for addressing the previous topics, the first one a simple piece-wise regression model trained on real data, the second one a Gaussian processes meta-model trained on computer simulation data and calibrated with respect to piece-wise regression data and the third one a detailed simulation model directly fitted to real data. The emphasis is put on the creation of the "black-box" meta-model through Gaussian processes regression technique with a radial basis function kernel, in order to establish a methodology suitable for the integrated use of multivariate real measured data and computer-based experimental data (DOE) obtained with detailed "white box" building energy models. The meta-model allows performing optimization, uncertainty and sensitivity analysis in an easier and more computationally efficient way than the original detailed simulation model. Further, the methodology presented can be extended to highly multivariate input and multiple output data, enabling its application to real-time building energy analysis for continuous commissioning (e.g. model predictive control, monitoring of energy consumption, building components performance durability, etc.) and event detection (e.g. peak power absorption, faults, etc.), in particular in the emerging field of smart grid and within district energy systems. In fact, one of the most important outcomes of the research is the creation of easily deployable, scalable and flexible tools to perform multi-objective, multi-scale and multi-period modeling. In the cases in which a detailed modeling of all buildings and

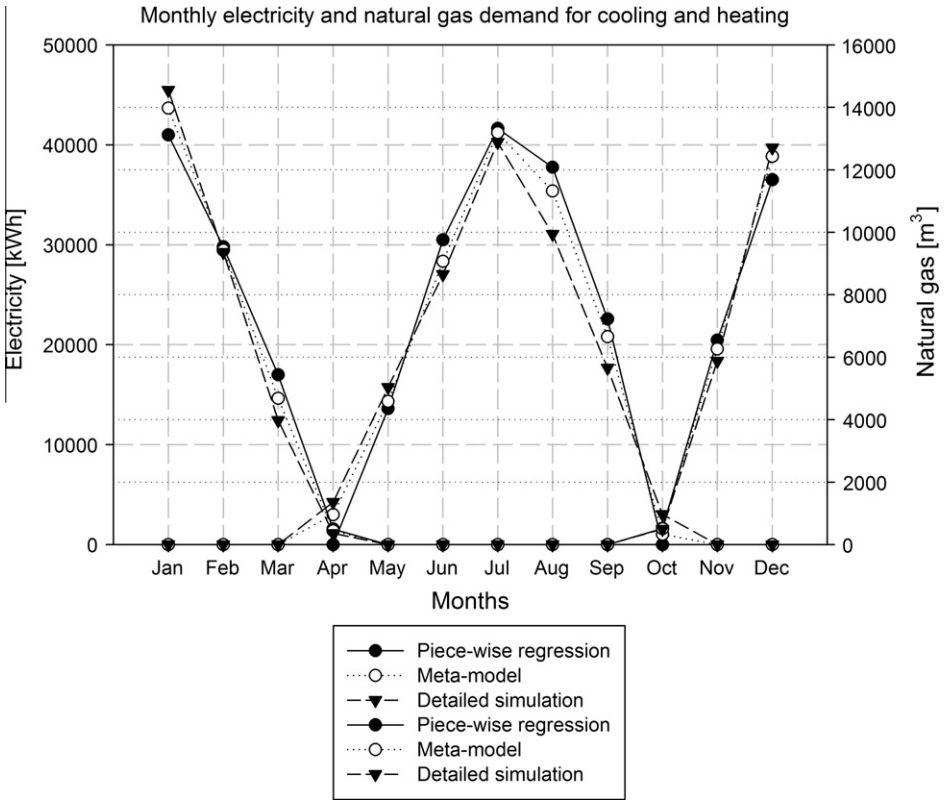

Fig. 8. Comparison between energy demand for heating and cooling predicted with piece-wise regression, GP meta-model and detailed model for reference meteorological year.

Table 9
Comparison of the global results obtained with the different models for a reference meteorological year.

Model	Electricity (cooling) (kWh)	Natural gas (heating) (m^3)
Piece-wise regression model	146,060	47,317
Meta-model	140,899	47,207
Detailed simulation model	139,048	47,328

activities is impractical and the research for optimal solutions, according to the selected performance criteria (one or more than one), can become infeasible, data-driven models represents clearly a possible solution. The idea of bridging the gap between data-driven and model-driven procedures and tools towards an integrated and unified approach seems to be the key point for a mature simulation based design methodology, focused not merely on the computational process itself but rather on the application and integration of algorithms for several different purposes.

In any case, a modeling strategy which uses a simplified physical approach, ''grey-box'', is preferable to a ''black-box'' one, not necessarily in terms of absolute performance (accuracy, robustness of results, etc.), but rather in terms of usability and transparency to the end-user.

For example, due to the success of state-space modeling approach for simulation, optimization and time-series forecasting, the integration of GP technique and state-space formulations (which have proven to be a good technique in several fields of application from simulation to control and forecasting) is one of the possible developments in the research,

A reflection on a ''grey-box'' approach able to address different scales and time resolutions of data with the same technique is fundamental and, in this case, more data are needed to obtain a useful reduced-order model, but the parameters can lead to a simplified physical interpretation of the underlying phenomena, increasing the confidence in the results.

Adopting a Bayesian framework in stochastic processes' modeling is fundamental and although this analysis framework has been rendered more accessible in the last years (through user-friendly tools), it is necessary to recognize the effort that this technique requires. GP technique, which assumes a Gaussian noise model in a Bayesian analysis, seem to be a good compromise between accuracy and computational cost.

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